```
COST IN U.S. DOLLARS                                    SINCE FILE      TOTAL
                                                           ENTRY    SESSION
FULL ESTIMATED COST                                       167.38     167.59

=> d his

     (FILE 'HOME' ENTERED AT 12:43:29 ON 14 JUN 2006)

     FILE 'REGISTRY' ENTERED AT 12:44:03 ON 14 JUN 2006
L1             STRUCTURE UPLOADED
L2           0 S L1
L3           0 S L1 FULL

=> file reg
COST IN U.S. DOLLARS                                    SINCE FILE      TOTAL
                                                           ENTRY    SESSION
FULL ESTIMATED COST                                       167.38     167.59

FILE 'REGISTRY' ENTERED AT 12:49:35 ON 14 JUN 2006
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STRUCTURE FILE UPDATES:   13 JUN 2006  HIGHEST RN 887650-39-7
DICTIONARY FILE UPDATES:  13 JUN 2006  HIGHEST RN 887650-39-7

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TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

*********************************************************************
*                                                                   *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added,   *
* effective March 20, 2005.  A new display format, IDERL, is now    *
* available and contains the CA role and document type information. *
*                                                                   *
*********************************************************************

Structure search iteration limits have been increased.  See HELP SLIMITS
for details.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10099830_2.str
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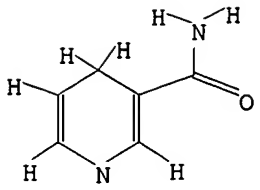

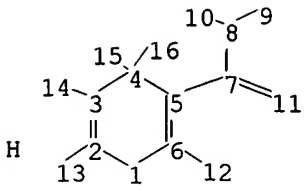

17

chain nodes :
7 8 9 10 11 12 13 14 15 16 17
ring nodes :
1 2 3 4 5 6
chain bonds :
2-13 3-14 4-15 4-16 5-7 6-12 7-8 7-11 8-9 8-10
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-11
exact bonds :
2-13 3-14 4-15 4-16 5-7 6-12 8-9 8-10

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS

L4 STRUCTURE UPLOADED

=> s l4 full
FULL SEARCH INITIATED 12:49:51 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 226903 TO ITERATE

100.0% PROCESSED 226903 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.02

L5 0 SEA SSS FUL L4

=>

---Logging off of STN---

=>
Executing the logoff script...

=> LOG Y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	166.94	334.53

STN INTERNATIONAL LOGOFF AT 12:50:07 ON 14 JUN 2006

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1642BJF

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page URLs for STN Seminar Schedule - N. America
NEWS 2		"Ask CAS" for self-help around the clock
NEWS 3	JAN 17	Pre-1988 INPI data added to MARPAT
NEWS 4	FEB 21	STN AnaVist, Version 1.1, lets you share your STN AnaVist visualization results
NEWS 5	FEB 22	The IPC thesaurus added to additional patent databases on STN
NEWS 6	FEB 22	Updates in EPFULL; IPC 8 enhancements added
NEWS 7	FEB 27	New STN AnaVist pricing effective March 1, 2006
NEWS 8	MAR 03	Updates in PATDPA; addition of IPC 8 data without attributes
NEWS 9	MAR 22	EMBASE is now updated on a daily basis
NEWS 10	APR 03	New IPC 8 fields and IPC thesaurus added to PATDPAFULL
NEWS 11	APR 03	Bibliographic data updates resume; new IPC 8 fields and IPC thesaurus added in PCTFULL
NEWS 12	APR 04	STN AnaVist $500 visualization usage credit offered
NEWS 13	APR 12	LINSPEC, learning database for INSPEC, reloaded and enhanced
NEWS 14	APR 12	Improved structure highlighting in FQHIT and QHIT display in MARPAT
NEWS 15	APR 12	Derwent World Patents Index to be reloaded and enhanced during second quarter; strategies may be affected
NEWS 16	MAY 10	CA/CAplus enhanced with 1900-1906 U.S. patent records
NEWS 17	MAY 11	KOREAPAT updates resume
NEWS 18	MAY 19	Derwent World Patents Index to be reloaded and enhanced
NEWS 19	MAY 30	IPC 8 Rolled-up Core codes added to CA/CAplus and USPATFULL/USPAT2
NEWS 20	MAY 30	The F-Term thesaurus is now available in CA/CAplus
NEWS 21	JUN 02	The first reclassification of IPC codes now complete in INPADOC
NEWS EXPRESS		FEBRUARY 15 CURRENT VERSION FOR WINDOWS IS V8.01a, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 19 DECEMBER 2005. V8.0 AND V8.01 USERS CAN OBTAIN THE UPGRADE TO V8.01a AT http://download.cas.org/express/v8.0-Discover/
NEWS HOURS		STN Operating Hours Plus Help Desk Availability
NEWS LOGIN		Welcome Banner and News Items
NEWS IPC8		For general information regarding STN implementation of IPC 8
NEWS X25		X.25 communication option no longer available after June 2006

Enter NEWS followed by the item number or name to see news on that specific topic.

```
* * * * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 14:30:32 ON 14 JUN 2006

=> file caplus
COST IN U.S. DOLLARS                                    SINCE FILE      TOTAL
                                                           ENTRY    SESSION
FULL ESTIMATED COST                                         0.21       0.21

FILE 'CAPLUS' ENTERED AT 14:30:42 ON 14 JUN 2006
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FILE COVERS 1907 - 14 Jun 2006  VOL 144 ISS 25
FILE LAST UPDATED: 13 Jun 2006  (20060613/ED)

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http://www.cas.org/infopolicy.html

=> s us 20030086933/pn
L1            1 US 20030086933/PN
                (US2003086933/PN)

=> sel rn
E1 THROUGH E45 ASSIGNED

=> file reg
COST IN U.S. DOLLARS                                    SINCE FILE      TOTAL
                                                           ENTRY    SESSION
FULL ESTIMATED COST                                         2.49       2.70

FILE 'REGISTRY' ENTERED AT 14:30:57 ON 14 JUN 2006
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STRUCTURE FILE UPDATES:   13 JUN 2006  HIGHEST RN 887650-39-7
DICTIONARY FILE UPDATES:  13 JUN 2006  HIGHEST RN 887650-39-7

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.
```

```
**********************************************************************
*                                                                    *
* The CA roles and document type information have been removed from  *
* the IDE default display format and the ED field has been added,    *
* effective March 20, 2005.  A new display format, IDERL, is now     *
* available and contains the CA role and document type information.  *
*                                                                    *
**********************************************************************

Structure search iteration limits have been increased.  See HELP SLIMITS
for details.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=> s e1-e45
             1 19132-12-8/BI
               (19132-12-8/RN)
             1 21919-05-1/BI
               (21919-05-1/RN)
             1 100-39-0/BI
               (100-39-0/RN)
             1 106-94-5/BI
               (106-94-5/RN)
             1 106047-77-2/BI
               (106047-77-2/RN)
             1 107-08-4/BI
               (107-08-4/RN)
             1 109942-74-7/BI
               (109942-74-7/RN)
             1 1120-71-4/BI
               (1120-71-4/RN)
             1 114554-11-9/BI
               (114554-11-9/RN)
             1 115503-79-2/BI
               (115503-79-2/RN)
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               (119643-82-2/RN)
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               OR 106047-77-2/BI OR 107-08-4/BI OR 109942-74-7/BI OR 1120-71-4/
               BI OR 114554-11-9/BI OR 115503-79-2/BI OR 119643-82-2/BI OR 12629
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               89080-16-0/BI OR 9037-41-6/BI OR 952-92-1/BI OR 97009-81-9/BI OR
               98-92-0/BI OR 99362-74-0/BI)

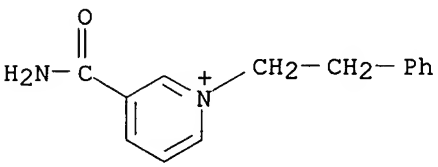
=> d 1-45

L2   ANSWER 1 OF 45  REGISTRY  COPYRIGHT 2006 ACS on STN
RN   667919-86-0  REGISTRY
ED   Entered STN:  26 Mar 2004
```

CN Dehydrogenase, reduced nicotinamide riboside (quinone) (9CI) (CA INDEX NAME)
OTHER NAMES:
CN Dihydronicotinamide riboside quinone oxidoreductase 2
CN Dihydronicotinamide riboside quinone reductase 2
CN Dihydronicotinamide riboside:quinone oxidoreductase
CN NQO2 oxidoreductase
CN NRH:quinone oxidoreductase
CN Quinone reductase 2
CN Reduced nicotinamide riboside (quinone) dehydrogenase
MF Unspecified
CI MAN
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

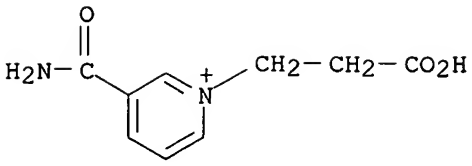
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
39 REFERENCES IN FILE CA (1907 TO DATE)
39 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 2 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **218443-93-7** REGISTRY
ED Entered STN: 29 Jan 1999
CN Pyridinium, 3-(aminocarbonyl)-1-(2-phenylethyl)-, iodide (9CI) (CA INDEX NAME)
MF C14 H15 N2 O . I
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL
CRN (761385-40-4)



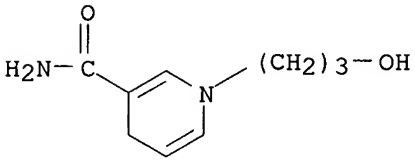
2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 3 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **218443-92-6** REGISTRY
ED Entered STN: 29 Jan 1999
CN Pyridinium, 3-(aminocarbonyl)-1-(2-carboxyethyl)-, iodide (9CI) (CA INDEX NAME)
MF C9 H11 N2 O3 . I
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL
CRN (717820-87-6)



2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

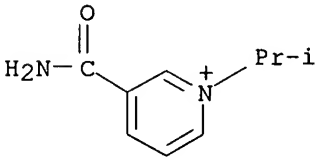
L2 ANSWER 4 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **218443-91-5** REGISTRY
ED Entered STN: 29 Jan 1999
CN 3-Pyridinecarboxamide, 1,4-dihydro-1-(3-hydroxypropyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C9 H14 N2 O2
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

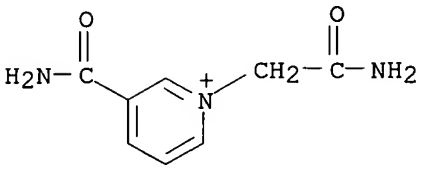
2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 5 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **218443-90-4** REGISTRY
ED Entered STN: 29 Jan 1999
CN Pyridinium, 3-(aminocarbonyl)-1-(1-methylethyl)-, bromide (9CI) (CA INDEX NAME)
MF C9 H13 N2 O . Br
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL
CRN (745779-44-6)



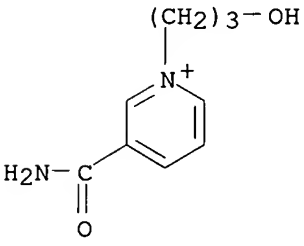
2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 6 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **218443-88-0** REGISTRY
ED Entered STN: 29 Jan 1999
CN Pyridinium, 3-(aminocarbonyl)-1-(2-amino-2-oxoethyl)-, iodide (9CI) (CA INDEX NAME)
MF C8 H10 N3 O2 . I
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL
CRN (66822-26-2)



3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

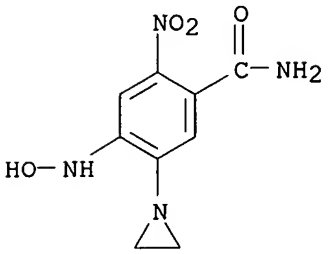
L2 ANSWER 7 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **126298-92-8** REGISTRY
ED Entered STN: 06 Apr 1990
CN Pyridinium, 3-(aminocarbonyl)-1-(3-hydroxypropyl)-, bromide (9CI) (CA INDEX NAME)
MF C9 H13 N2 O2 . Br
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL
CRN (83643-85-0)



4 REFERENCES IN FILE CA (1907 TO DATE)
4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 8 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **119643-82-2** REGISTRY
ED Entered STN: 17 Mar 1989
CN Benzamide, 5-(1-aziridinyl)-4-(hydroxyamino)-2-nitro- (9CI) (CA INDEX NAME)

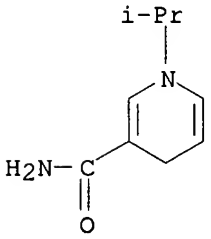
FS 3D CONCORD
MF C9 H10 N4 O4
SR CA
LC STN Files: CA, CAPLUS, MEDLINE, TOXCENTER, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

13 REFERENCES IN FILE CA (1907 TO DATE)
13 REFERENCES IN FILE CAPLUS (1907 TO DATE)

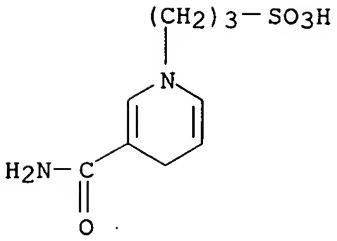
L2 ANSWER 9 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **115503-79-2** REGISTRY
ED Entered STN: 30 Jul 1988
CN 3-Pyridinecarboxamide, 1,4-dihydro-1-(1-methylethyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C9 H14 N2 O
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

5 REFERENCES IN FILE CA (1907 TO DATE)
5 REFERENCES IN FILE CAPLUS (1907 TO DATE)

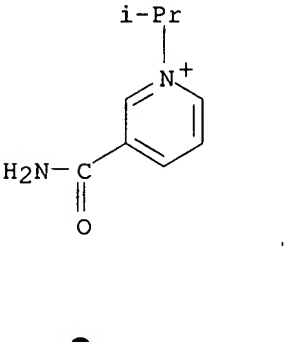
L2 ANSWER 10 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **114554-11-9** REGISTRY
ED Entered STN: 21 May 1988
CN 1(4H)-Pyridinepropanesulfonic acid, 3-(aminocarbonyl)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1(4H)-Pyridinepropanesulfonic acid, 3-carbamoyl- (6CI)
FS 3D CONCORD
MF C9 H14 N2 O4 S
SR CAOLD
LC STN Files: CA, CAOLD, CAPLUS, TOXCENTER, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

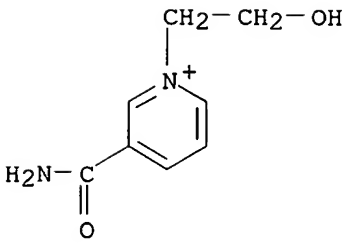
3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L2 ANSWER 11 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **109942-74-7** REGISTRY
ED Entered STN: 22 Aug 1987
CN Pyridinium, 3-(aminocarbonyl)-1-(1-methylethyl)-, iodide (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 3-Carbamoyl-1-isopropylpyridinium iodide (6CI)
MF C9 H13 N2 O . I
SR CAOLD
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)
CRN (745779-44-6)



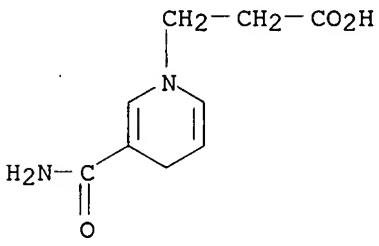
5 REFERENCES IN FILE CA (1907 TO DATE)
5 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L2 ANSWER 12 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **106047-77-2** REGISTRY
ED Entered STN: 10 Jan 1987
CN Pyridinium, 3-(aminocarbonyl)-1-(2-hydroxyethyl)-, iodide (9CI) (CA INDEX NAME)
MF C8 H11 N2 O2 . I
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL
CRN (66822-21-7)



4 REFERENCES IN FILE CA (1907 TO DATE)
4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

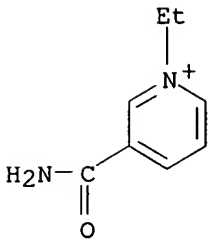
L2 ANSWER 13 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **99362-74-0** REGISTRY
ED Entered STN: 07 Dec 1985
CN 1(4H)-Pyridinepropanoic acid, 3-(aminocarbonyl)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1(4H)-Pyridinepropionic acid, 3-carbamoyl- (6CI)
FS 3D CONCORD
MF C9 H12 N2 O3
SR CAOLD
LC STN Files: CA, CAOLD, CAPLUS, TOXCENTER, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

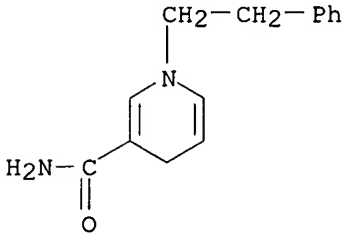
3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L2 ANSWER 14 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **97009-81-9** REGISTRY
ED Entered STN: 01 Jul 1985
CN Pyridinium, 3-(aminocarbonyl)-1-ethyl-, iodide (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 3-Carbamoyl-1-ethylpyridinium iodide (6CI)
CN Pyridinium, 3-carbamyl-1-ethyl-, iodide (4CI)
MF C8 H11 N2 O . I
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)
CRN (71413-64-4)



12 REFERENCES IN FILE CA (1907 TO DATE)
12 REFERENCES IN FILE CAPLUS (1907 TO DATE)
3 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

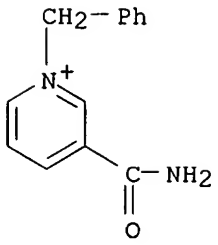
L2 ANSWER 15 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **89080-16-0** REGISTRY
ED Entered STN: 16 Nov 1984
CN 3-Pyridinecarboxamide, 1,4-dihydro-1-(2-phenylethyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C14 H16 N2 O
LC STN Files: BEILSTEIN*, CA, CAPLUS, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1907 TO DATE)
4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

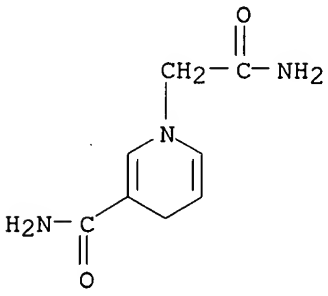
L2 ANSWER 16 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **72306-81-1** REGISTRY
ED Entered STN: 16 Nov 1984
CN Pyridinium, 3-(aminocarbonyl)-1-(phenylmethyl)-, iodide (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1-Benzyl-3-carbamoylpyridinium iodide (6CI, 7CI)
MF C13 H13 N2 O . I
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)
CRN (16183-83-8)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

5 REFERENCES IN FILE CA (1907 TO DATE)
5 REFERENCES IN FILE CAPLUS (1907 TO DATE)
2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L2 ANSWER 17 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **64881-21-6** REGISTRY
ED Entered STN: 16 Nov 1984
CN 1(4H)-Pyridineacetamide, 3-(aminocarbonyl)- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN 1-Carbamoylmethyl-1,4-dihydronicotinamide
CN Caricotamide
CN EP 0152R
FS 3D CONCORD
MF C8 H11 N3 O2
LC STN Files: BEILSTEIN*, CA, CAPLUS, TOXCENTER, USAN, USPATFULL
(*File contains numerically searchable property data)

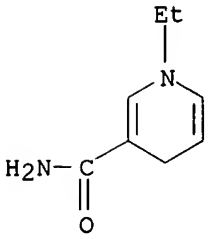


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1907 TO DATE)
9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 18 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **58880-44-7** REGISTRY
ED Entered STN: 16 Nov 1984
CN 3-Pyridinecarboxamide, 1-ethyl-1,4-dihydro- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN N-Ethyl-1,4-dihydronicotinamide
FS 3D CONCORD
MF C8 H12 N2 O
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL

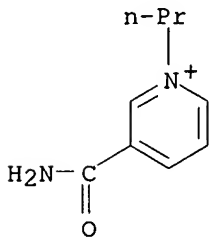
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

8 REFERENCES IN FILE CA (1907 TO DATE)
8 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 19 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **52047-79-7** REGISTRY
ED Entered STN: 16 Nov 1984
CN Pyridinium, 3-(aminocarbonyl)-1-propyl-, bromide (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Pyridinium, 3-carbamoyl-1-propyl-, bromide (6CI)
OTHER NAMES:
CN 3-Carbamoyl-1-propylpyridinium bromide
MF C9 H13 N2 O . Br
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CHEMCATS, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)
CRN (13309-33-6)

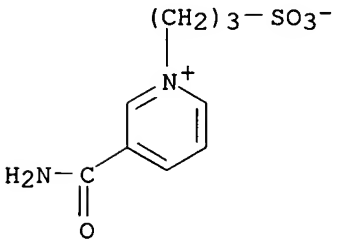


● Br^-

15 REFERENCES IN FILE CA (1907 TO DATE)
15 REFERENCES IN FILE CAPLUS (1907 TO DATE)
4 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L2 ANSWER 20 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **51652-08-5** REGISTRY
ED Entered STN: 16 Nov 1984
CN Pyridinium, 3-(aminocarbonyl)-1-(3-sulfopropyl)-, inner salt (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 3-Carbamoyl-1-(3-sulfopropyl)pyridinium hydroxide, inner salt (6CI)
CN Pyridinium, 3-(aminocarbonyl)-1-(3-sulfopropyl)-, hydroxide, inner salt
FS 3D CONCORD
MF C9 H12 N2 O4 S
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, CHEMLIST, MSDS-OHS, TOXCENTER, USPATFULL

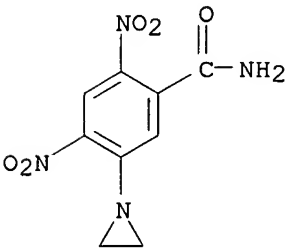
(*File contains numerically searchable property data)
Other Sources: EINECS**
(**Enter CHEMLIST File for up-to-date regulatory information)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

11 REFERENCES IN FILE CA (1907 TO DATE)
11 REFERENCES IN FILE CAPLUS (1907 TO DATE)
2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L2 ANSWER 21 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **21919-05-1** REGISTRY
ED Entered STN: 16 Nov 1984
CN Benzamide, 5-(1-aziridinyl)-2,4-dinitro- (8CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
CN 2,4-Dinitro-5-ethyleneiminobenzamide
CN 2,4-Dinitroethyleneiminobenzamide
CN 5-(1-Aziridinyl)-2,4-dinitrobenzamide
CN 5-Aziridino-2,4-dinitrobenzamide
CN 5-Aziridinyl-2,4-dinitrobenzamide
CN CB 1954
CN NSC 115829
CN Tretazicar
MF C9 H8 N4 O5
LC STN Files: ADISNEWS, ANABSTR, BEILSTEIN*, BIOSIS, BIOTECHNO, CA, CAPLUS, CASREACT, CHEMCATS, CIN, CSCHEM, DDFU, DRUGU, EMBASE, IMSDRUGNEWS, IMSRESEARCH, MEDLINE, PROMT, PROUSDDR, RTECS*, TOXCENTER, USAN, USPAT2, USPATFULL
(*File contains numerically searchable property data)



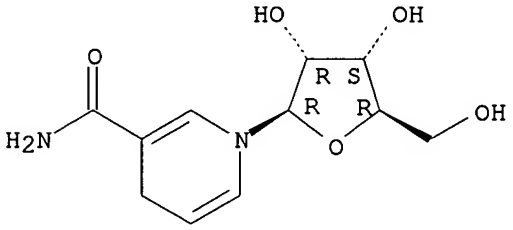
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

176 REFERENCES IN FILE CA (1907 TO DATE)
5 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
176 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 22 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **19132-12-8** REGISTRY

ED Entered STN: 16 Nov 1984
CN 3-Pyridinecarboxamide, 1,4-dihydro-1-β-D-ribofuranosyl- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Nicotinamide, 1,4-dihydro-1-β-D-ribofuranosyl- (6CI, 7CI, 8CI)
OTHER NAMES:
CN β-Reduced nicotinamide ribonucleoside
CN Reduced nicotinamide riboside
FS STEREOSEARCH
MF C11 H16 N2 O5
CI COM
LC STN Files: BEILSTEIN*, BIOSIS, CA, CAOLD, CAPLUS, TOXCENTER, USPATFULL
    (*File contains numerically searchable property data)

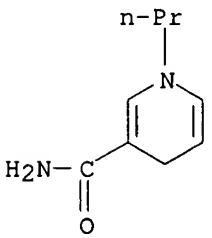
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

16 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
16 REFERENCES IN FILE CAPLUS (1907 TO DATE)
4 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

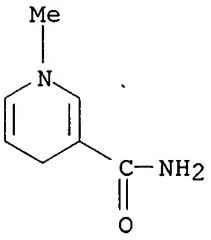
L2 ANSWER 23 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **17750-24-2** REGISTRY
ED Entered STN: 16 Nov 1984
CN 3-Pyridinecarboxamide, 1,4-dihydro-1-propyl- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Nicotinamide, 1,4-dihydro-1-propyl- (6CI, 7CI, 8CI)
OTHER NAMES:
CN 1,4-Dihydro-N1-propylnicotinamide
CN 1-n-Propyl-1,4-dihydronicotinamide
CN 1-Propyl-1,4-dihydronicotinamide
CN N-Propyldihydronicotinamide
CN N1-(n-Propyl)-1,4-dihydronicotinamide
FS 3D CONCORD
MF C9 H14 N2 O
LC STN Files: BEILSTEIN*, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, TOXCENTER, USPATFULL
    (*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

96 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
96 REFERENCES IN FILE CAPLUS (1907 TO DATE)
15 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L2 ANSWER 24 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **17750-23-1** REGISTRY
ED Entered STN: 16 Nov 1984
CN 3-Pyridinecarboxamide, 1,4-dihydro-1-methyl- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Nicotinamide, 1,4-dihydro-1-methyl- (6CI, 8CI)
OTHER NAMES:
CN 1,4-Dihydro-1-methylnicotinamide
CN 1,4-Dihydro-N-methylnicotinamide
CN 1-Methyl-1,4-dihydronicotinamide
CN 3-Carbamoyl-1,4-dihydro-1-methylpyridine
CN N-Methyl-1,4-dihydronicotinamide
FS 3D CONCORD
MF C7 H10 N2 O
CI COM
LC STN Files: BEILSTEIN*, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, IFICDB, IFIPAT, IFIUDB, MEDLINE, TOXCENTER, USPAT2, USPATFULL
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

107 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
107 REFERENCES IN FILE CAPLUS (1907 TO DATE)
3 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L2 ANSWER 25 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **17376-04-4** REGISTRY
ED Entered STN: 16 Nov 1984
CN Benzene, (2-iodoethyl)- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
CN (2-Iodoethyl)benzene
CN β-Phenethyl iodide
CN β-Phenylethyl iodide
CN 1-Iodo-2-phenylethane
CN 2-Phenylethyl iodide
CN Phenethyl iodide
FS 3D CONCORD
MF C8 H9 I
CI COM
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, CSCHEM, DETHERM*, GMELIN*, SPECINFO, TOXCENTER, USPAT2, USPATFULL
(*File contains numerically searchable property data)
Other Sources: NDSL**, TSCA**

(**Enter CHEMLIST File for up-to-date regulatory information)

ICH_2-CH_2-Ph

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

281 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
282 REFERENCES IN FILE CAPLUS (1907 TO DATE)
15 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

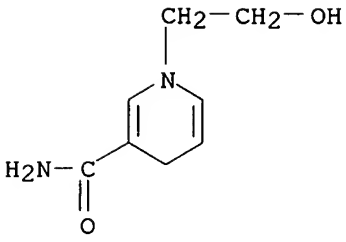
L2 ANSWER 26 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **9037-41-6** REGISTRY
ED Entered STN: 16 Nov 1984
CN Reductase, nitro- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN 2,4,6-Trinitrotoluene nitroreductase
CN 3-Nitrophenol reductase
CN 4-Nitrobiphenyl reductase
CN Aromatic nitroreductase
CN Dinitropyrene nitroreductase
CN Nitrobenzene nitroreductase
CN Nitrobenzene reductase
CN Nitrobenzoic acid reductase
CN Nitrophenol reductase
CN Nitroreductase
CN Nitroreductase (NADH)
CN PETN reductase
CN TNT nitroreductase
MF Unspecified
CI MAN
LC STN Files: ADISNEWS, AGRICOLA, BIOSIS, BIOTECHNO, CA, CAPLUS, CASREACT, CIN, EMBASE, PIRA, PROMT, TOXCENTER, USPAT2, USPATFULL

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

679 REFERENCES IN FILE CA (1907 TO DATE)
11 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
680 REFERENCES IN FILE CAPLUS (1907 TO DATE)

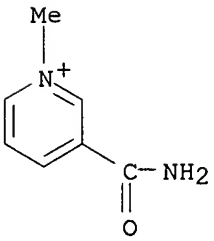
L2 ANSWER 27 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **7145-37-1** REGISTRY
ED Entered STN: 16 Nov 1984
CN 3-Pyridinecarboxamide, 1,4-dihydro-1-(2-hydroxyethyl)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Nicotinamide, 1,4-dihydro-1-(2-hydroxyethyl)- (7CI, 8CI)
OTHER NAMES:
CN NSC 74259
FS 3D CONCORD
MF C8 H12 N2 O2
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

6 REFERENCES IN FILE CA (1907 TO DATE)
6 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

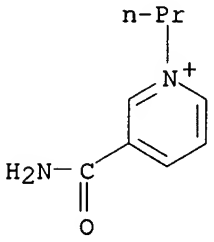
L2 ANSWER 28 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **6456-44-6** REGISTRY
ED Entered STN: 16 Nov 1984
CN Pyridinium, 3-(aminocarbonyl)-1-methyl-, iodide (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 3-Carbamoyl-1-methylpyridinium iodide (6CI, 7CI)
CN Pyridinium, 3-carbamoyl-1-methyl-, iodide (8CI)
CN Pyridinium, 3-carbamyl-1-methyl-, iodide (4CI)
OTHER NAMES:
CN 1-Methylnicotinamide iodide
CN Nicotinamide methiodide
MF C7 H9 N2 O . I
CI COM
SR CA
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMLIST, CSCHEM, GMELIN*, RTECS*, TOXCENTER, USPAT2, USPATFULL
(*File contains numerically searchable property data)
Other Sources: EINECS**
(**Enter CHEMLIST File for up-to-date regulatory information)
CRN (3106-60-3)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

104 REFERENCES IN FILE CA (1907 TO DATE)
104 REFERENCES IN FILE CAPLUS (1907 TO DATE)
19 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L2 ANSWER 29 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **5463-59-2** REGISTRY
ED Entered STN: 16 Nov 1984
CN Pyridinium, 3-(aminocarbonyl)-1-propyl-, iodide (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 3-Carbamoyl-1-propylpyridinium iodide (6CI, 7CI)
CN Pyridinium, 3-carbamoyl-1-propyl-, iodide (8CI)
MF C9 H13 N2 O . I
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)
CRN (13309-33-6)

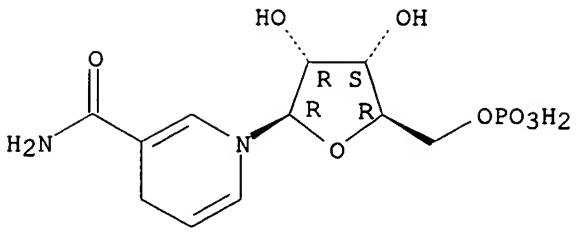


● I^-

18 REFERENCES IN FILE CA (1907 TO DATE)
18 REFERENCES IN FILE CAPLUS (1907 TO DATE)
4 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L2 ANSWER 30 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **4229-56-5** REGISTRY
ED Entered STN: 16 Nov 1984
CN 3-Pyridinecarboxamide, 1,4-dihydro-1-(5-O-phosphono-β-D-ribofuranosyl)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Nicotinamide, 1,4-dihydro-1-β-D-ribofuranosyl-, 5'-(dihydrogen phosphate) (8CI)
CN Nicotinamide, 1,4-dihydro-1-β-D-ribofuranosyl-, 5'-phosphate (7CI)
OTHER NAMES:
CN β-NMNH
CN 1,4-Dihydronicotinamide mononucleotide
CN 1,4-Dihydronicotinamide ribonucleotide
CN Nicotinamide ribonucleotide, reduced
CN NMNH
CN NMNH2
CN Reduced nicotinamide mononucleotide
CN Reduced nicotinamide ribonucleotide
FS STEREOSEARCH
MF C11 H17 N2 O8 P
CI COM
LC STN Files: AGRICOLA, BEILSTEIN*, CA, CAOLD, CAPLUS, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)

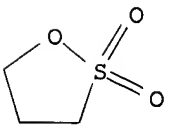
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

77 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
77 REFERENCES IN FILE CAPLUS (1907 TO DATE)
4 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

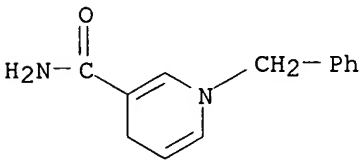
L2 ANSWER 31 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **1120-71-4** REGISTRY
ED Entered STN: 16 Nov 1984
CN 1,2-Oxathiolane, 2,2-dioxide (8CI, 9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1-Propanesulfonic acid, 3-hydroxy-, γ-sultone (6CI)
OTHER NAMES:
CN γ-Propane sultone
CN 1,3-Propane sultone
CN 1,3-Trimethylene sultone
CN 3-Hydroxy-1-propanesulfonic acid γ-sultone
CN 3-Hydroxy-1-propanesulfonic acid sultone
CN NSC 42386
CN Propane sultone
CN Propyl sultone
FS 3D CONCORD
MF C3 H6 O3 S
CI COM
LC STN Files: AGRICOLA, ANABSTR, BEILSTEIN*, BIOSIS, BIOTECHNO, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, CHEMSAFE, CIN, CSCHEM, CSNB, DETHERM*, EMBASE, ENCOMPPAT, ENCOMPPAT2, GMELIN*, HSDB*, IFICDB, IFIPAT, IFIUDB, MEDLINE, MSDS-OHS, PROMT, PS, RTECS*, SPECINFO, TOXCENTER, ULIDAT, USPAT2, USPATFULL
(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1761 REFERENCES IN FILE CA (1907 TO DATE)
383 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
1765 REFERENCES IN FILE CAPLUS (1907 TO DATE)
31 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L2 ANSWER 32 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **952-92-1** REGISTRY
ED Entered STN: 16 Nov 1984
CN 3-Pyridinecarboxamide, 1,4-dihydro-1-(phenylmethyl)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Nicotinamide, 1-benzyl-1,4-dihydro- (6CI, 7CI, 8CI)
OTHER NAMES:
CN 1,4-Dihydro-1-(phenylmethyl)-3-pyridinecarboxamide
CN 1,4-Dihydro-N-benzylnicotinamide
CN 1-Benzyl-1,4-dihydronicotinamide
CN 1-Benzyl-3-carbamido-1,4-dihydropyridine
CN 1-Benzyl-3-carbamoyl-1,4-dihydropyridine
CN BNAH
CN N-Benzyl-1,4-dihydronicotinamide
CN N-Benzyl-3-carbamoyl-1,4-dihydropyridine
CN N-Benzyldihydronicotinamide
CN NSC 26899
FS 3D CONCORD
DR 174307-50-7, 84062-23-7
MF C13 H14 N2 O
CI COM
LC STN Files: AGRICOLA, BEILSTEIN*, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CSCHEM, GMELIN*, IFICDB, IFIPAT, IFIUDB, MEDLINE, PIRA, PROMT, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

584 REFERENCES IN FILE CA (1907 TO DATE)
10 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
584 REFERENCES IN FILE CAPLUS (1907 TO DATE)
31 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L2 ANSWER 33 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **627-18-9** REGISTRY
ED Entered STN: 16 Nov 1984
CN 1-Propanol, 3-bromo- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
CN 1-Bromo-3-hydroxypropane
CN 1-Bromo-3-propanol
CN 3-Bromo-1-propanol
CN 3-Bromopropyl alcohol
CN 3-Hydroxypropyl bromide
CN Trimethylene bromohydrin
FS 3D CONCORD
MF C3 H7 Br O
CI COM
LC STN Files: BEILSTEIN*, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, CSCHEM, EMBASE, GMELIN*, IFICDB, IFIPAT, IFIUDB, PS, RTECS*, SPECINFO, SYNTHLINE, TOXCENTER, USPAT2, USPATFULL
(*File contains numerically searchable property data)

Other Sources: EINECS**, NDSL**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)

Br—CH_2—CH_2—CH_2—OH

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1404 REFERENCES IN FILE CA (1907 TO DATE)
18 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
1409 REFERENCES IN FILE CAPLUS (1907 TO DATE)
8 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L2 ANSWER 34 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **624-76-0** REGISTRY
ED Entered STN: 16 Nov 1984
CN Ethanol, 2-iodo- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
CN 2-Iodoethanol
CN Ethylene iodohydrin
CN Iodoethanol
CN NSC 85227
FS 3D CONCORD
MF C2 H5 I O
CI COM
LC STN Files: BEILSTEIN*, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, CSCHEM, DETHERM*, IFICDB, IFIPAT, IFIUDB, RTECS*, SPECINFO, SYNTHLINE, TOXCENTER, USPAT2, USPATFULL
(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)

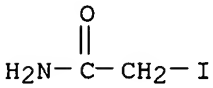
I—CH_2—CH_2—OH

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

477 REFERENCES IN FILE CA (1907 TO DATE)
7 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
477 REFERENCES IN FILE CAPLUS (1907 TO DATE)
7 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L2 ANSWER 35 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **144-48-9** REGISTRY
ED Entered STN: 16 Nov 1984
CN Acetamide, 2-iodo- (8CI, 9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Acetamide, iodo- (6CI)
OTHER NAMES:
CN α-Iodoacetamide
CN 2-Iodoacetamide
CN Iodoacetamide
CN Monoiodoacetamide
CN NSC 9581
CN Surauto
FS 3D CONCORD
MF C2 H4 I N O
CI COM
LC STN Files: AGRICOLA, AQUIRE, BEILSTEIN*, BIOSIS, BIOTECHNO, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, CSCHEM, DDFU, DRUGU,

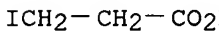
EMBASE, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, MSDS-OHS, NAPRALERT, PIRA, PROMT, RTECS*, SCISEARCH, SYNTHLINE, TOXCENTER, USPAT2, USPATFULL, VETU
(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1651 REFERENCES IN FILE CA (1907 TO DATE)
46 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
1654 REFERENCES IN FILE CAPLUS (1907 TO DATE)
80 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L2 ANSWER 36 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **141-76-4** REGISTRY
ED Entered STN: 16 Nov 1984
CN Propanoic acid, 3-iodo- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Propionic acid, 3-iodo- (6CI, 7CI, 8CI)
OTHER NAMES:
CN β-Iodopropionic acid
CN 3-Iodopropanoic acid
CN 3-Iodopropionic acid
CN NSC 2124
FS 3D CONCORD
MF C3 H5 I O2
CI COM
LC STN Files: ANABSTR, BEILSTEIN*, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, CSCHEM, GMELIN*, MSDS-OHS, RTECS*, SPECINFO, TOXCENTER, USPAT2, USPATFULL
(*File contains numerically searchable property data)
Other Sources: EINECS**, NDSL**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)

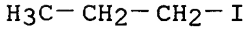


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

183 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
183 REFERENCES IN FILE CAPLUS (1907 TO DATE)
17 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L2 ANSWER 37 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **107-08-4** REGISTRY
ED Entered STN: 16 Nov 1984
CN Propane, 1-iodo- (8CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
CN 1-Iodopropane
CN n-Propyl iodide
CN Propane iodide
CN Propyl iodide
FS 3D CONCORD
MF C3 H7 I

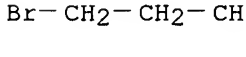
CI COM
LC STN Files: AGRICOLA, ANABSTR, BEILSTEIN*, BIOSIS, BIOTECHNO, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, CHEMSAFE, CSCHEM, DETHERM*, EMBASE, GMELIN*, IFICDB, IFIPAT, IFIUDB, MEDLINE, MRCK*, MSDS-OHS, NAPRALERT, PIRA, PROMT, PS, RTECS*, SPECINFO, SYNTHLINE, TOXCENTER, TULSA, USPAT2, USPATFULL, VTB
(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3224 REFERENCES IN FILE CA (1907 TO DATE)
13 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
3230 REFERENCES IN FILE CAPLUS (1907 TO DATE)
5 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L2 ANSWER 38 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **106-94-5** REGISTRY
ED Entered STN: 16 Nov 1984
CN Propane, 1-bromo- (8CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
CN 1-Bromopropane
CN 1-Propyl bromide
CN Ascusol MC
CN Leksol
CN n-Propyl bromide
CN Propyl bromide
FS 3D CONCORD
MF C3 H7 Br
CI COM
LC STN Files: AGRICOLA, ANABSTR, AQUIRE, BEILSTEIN*, BIOSIS, BIOTECHNO, CA, CAOLD, CAPLUS, CASREACT, CBNB, CHEMCATS, CHEMINFORMRX, CHEMLIST, CHEMSAFE, CIN, CSCHEM, CSNB, DETHERM*, EMBASE, GMELIN*, HSDB*, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, MRCK*, MSDS-OHS, NAPRALERT, PIRA, PROMT, PS, RTECS*, SCISEARCH, SPECINFO, SYNTHLINE, TOXCENTER, USPAT2, USPATFULL, VTB
(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)

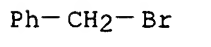


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4243 REFERENCES IN FILE CA (1907 TO DATE)
46 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
4250 REFERENCES IN FILE CAPLUS (1907 TO DATE)
5 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L2 ANSWER 39 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **100-39-0** REGISTRY
ED Entered STN: 16 Nov 1984
CN Benzene, (bromomethyl)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Toluene, α-bromo- (8CI)

OTHER NAMES:
CN (Bromomethyl)benzene
CN (Bromophenyl)methane
CN α-Bromotoluene
CN ω-Bromotoluene
CN Benzyl bromide
CN NSC 8041
CN Phenylmethyl bromide
FS 3D CONCORD
MF C7 H7 Br
CI COM
LC STN Files: AGRICOLA, ANABSTR, BEILSTEIN*, BIOSIS, BIOTECHNO, CA, CAOLD, CAPLUS, CASREACT, CBNB, CHEMCATS, CHEMINFORMRX, CHEMLIST, CIN, CSCHEM, DETHERM*, EMBASE, GMELIN*, HSDB*, IFICDB, IFIPAT, IFIUDB, MEDLINE, MRCK*, MSDS-OHS, PIRA, PROMT, PS, RTECS*, SPECINFO, SYNTHLINE, TOXCENTER, ULIDAT, USPAT2, USPATFULL
(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)

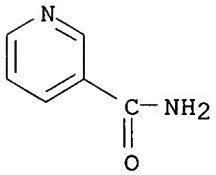


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

13933 REFERENCES IN FILE CA (1907 TO DATE)
106 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
13983 REFERENCES IN FILE CAPLUS (1907 TO DATE)
6 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L2 ANSWER 40 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **98-92-0** REGISTRY
ED Entered STN: 16 Nov 1984
CN 3-Pyridinecarboxamide (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Nicotinamide (8CI)
OTHER NAMES:
CN β-Pyridinecarboxamide
CN 3-(Aminocarbonyl)pyridine
CN 3-Amidopyridine
CN 3-Carbamoylpyridine
CN 3-Pyridinecarboxylic acid amide
CN Aminicotin
CN Benicot
CN Delonin Amide
CN Dipegyl
CN m-(Aminocarbonyl)pyridine
CN NAM
CN Niacinamide
CN Niavit PP
CN Nicamina
CN Nicamindon
CN Nicasir
CN Nicobion
CN Nicofort
CN Nicosan 2
CN Nicosylamide
CN Nicotilamide
CN Nicotine acid amide
CN Nicotinic acid amide
CN Nicotinic amide
CN Nicotylamide

CN Nicovit
CN Nicovitina
CN Nictoamide
CN Niocinamide
CN Niozymin
CN NSC 13128
CN NSC 27452
CN Papulex
CN Pelmin
CN Pelmine
CN Pelonin amide
CN Vi-Nicotyl
CN Vitamin B
CN Vitamin B3
FS 3D CONCORD
DR 123574-63-0, 37321-14-5, 78731-47-2
MF C6 H6 N2 O
CI COM
LC STN Files: ADISINSIGHT, ADISNEWS, AGRICOLA, ANABSTR, AQUIRE, BEILSTEIN*, BIOSIS, BIOTECHNO, CA, CABA, CAOLD, CAPLUS, CASREACT, CBNB, CHEMCATS, CHEMINFORMRX, CHEMLIST, CIN, CSCHEM, CSNB, DDFU, DETHERM*, DRUGU, EMBASE, GMELIN*, HSDB*, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, MRCK*, MSDS-OHS, NAPRALERT, PHAR, PIRA, PROMT, PS, RTECS*, SPECINFO, TOXCENTER, USAN, USPAT2, USPATFULL, VTB
(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**, WHO
(**Enter CHEMLIST File for up-to-date regulatory information)

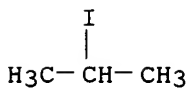


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9281 REFERENCES IN FILE CA (1907 TO DATE)
409 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
9303 REFERENCES IN FILE CAPLUS (1907 TO DATE)
9 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L2 ANSWER 41 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **75-30-9** REGISTRY
ED Entered STN: 16 Nov 1984
CN Propane, 2-iodo- (8CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
CN 1-Methylethyl iodide
CN 2-Iodopropane
CN 2-Propyl iodide
CN Isopropyl iodide
CN sec-Propyl iodide
FS 3D CONCORD
MF C3 H7 I
CI COM
LC STN Files: ANABSTR, BEILSTEIN*, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, CHEMSAFE, CSCHEM, DETHERM*, GMELIN*, IFICDB, IFIPAT, IFIUDB, MEDLINE, MRCK*, MSDS-OHS, PS, RTECS*, SPECINFO, SYNTHLINE, TOXCENTER, USPAT2, USPATFULL
(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**

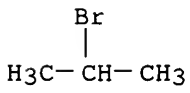
(**Enter CHEMLIST File for up-to-date regulatory information)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2962 REFERENCES IN FILE CA (1907 TO DATE)
7 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
2967 REFERENCES IN FILE CAPLUS (1907 TO DATE)
4 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L2 ANSWER 42 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **75-26-3** REGISTRY
ED Entered STN: 16 Nov 1984
CN Propane, 2-bromo- (8CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
CN 2-Bromopropane
CN Isopropyl bromide
CN sec-Propyl bromide
FS 3D CONCORD
MF C3 H7 Br
CI COM
LC STN Files: AGRICOLA, ANABSTR, BEILSTEIN*, BIOSIS, BIOTECHNO, CA, CAOLD, CAPLUS, CASREACT, CBNB, CHEMCATS, CHEMINFORMRX, CHEMLIST, CHEMSAFE, CIN, CSCHEM, CSNB, DETHERM*, EMBASE, GMELIN*, HSDB*, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, MRCK*, MSDS-OHS, PROMT, PS, RTECS*, SCISEARCH, SPECINFO, SYNTHLINE, TOXCENTER, ULIDAT, USPAT2, USPATFULL
(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)

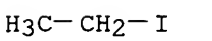


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3397 REFERENCES IN FILE CA (1907 TO DATE)
16 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
3407 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L2 ANSWER 43 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **75-03-6** REGISTRY
ED Entered STN: 16 Nov 1984
CN Ethane, iodo- (8CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
CN Ethyl iodide
CN Hydriodic ether
CN Iodoethane
CN Monoiodoethane
CN NSC 8825
FS 3D CONCORD
MF C2 H5 I
CI COM
LC STN Files: AGRICOLA, ANABSTR, BEILSTEIN*, BIOSIS, BIOTECHNO, CA, CAOLD,

CAPLUS, CASREACT, CBNB, CHEMCATS, CHEMINFORMRX, CHEMLIST, CIN, CSCHEM, CSNB, DETHERM*, EMBASE, ENCOMPLIT, ENCOMPLIT2, ENCOMPPAT, ENCOMPPAT2, GMELIN*, IFICDB, IFIPAT, IFIUDB, MEDLINE, MRCK*, MSDS-OHS, NAPRALERT, PIRA, PROMT, PS, RTECS*, SPECINFO, TOXCENTER, USPAT2, USPATFULL, VTB
(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)



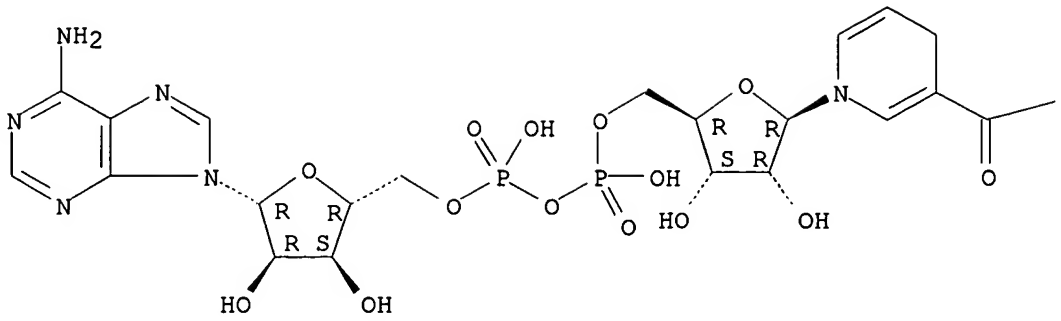
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

6901 REFERENCES IN FILE CA (1907 TO DATE)
74 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
6923 REFERENCES IN FILE CAPLUS (1907 TO DATE)
6 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L2 ANSWER 44 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **58-68-4** REGISTRY
ED Entered STN: 16 Nov 1984
CN Adenosine 5"-(trihydrogen diphosphate), P'→5'-ester with 1,4-dihydro-1-β-D-ribofuranosyl-3-pyridinecarboxamide (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Adenosine 5'-(trihydrogen pyrophosphate), 5'→5'-ester with 1,4-dihydro-1-β-D-ribofuranosylnicotinamide (8CI)
CN Adenosine pyrophosphate, 5'→5'-ester with 1,4-dihydro-1-β-D-ribofuranosylnicotinamide (7CI)
OTHER NAMES:
CN β-DPNH
CN β-NADH
CN 1,4-Dihydronicotinamide adenine dinucleotide
CN Codehydrase I, reduced
CN Codehydrogenase I, reduced
CN Coenzyme I, reduced
CN Cozymase I, reduced
CN Dihydrocodehydrogenase I
CN Dihydrocozymase
CN Dihydronicotinamide adenine dinucleotide
CN Dihydronicotinamide mononucleotide
CN DPNH
CN ENADA
CN NADH
CN NADH2
CN Nicotinamide-adenine dinucleotide, reduced
CN Reduced codehydrogenase I
CN Reduced diphosphopyridine nucleotide
CN Reduced nicotinamide adenine diphosphate
CN Reduced nicotinamide-adenine dinucleotide
FS STEREOSEARCH
DR 443892-10-2
MF C21 H29 N7 O14 P2
CI COM
LC STN Files: ADISNEWS, AGRICOLA, ANABSTR, BEILSTEIN*, BIOSIS, BIOTECHNO, CA, CABA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMLIST, CIN, CSCHEM, DDFU, DRUGU, EMBASE, GMELIN*, IFICDB, IFIPAT, IFIUDB, MRCK*, PIRA, PROMT, TOXCENTER, USPAT2, USPATFULL
(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

—NH_2

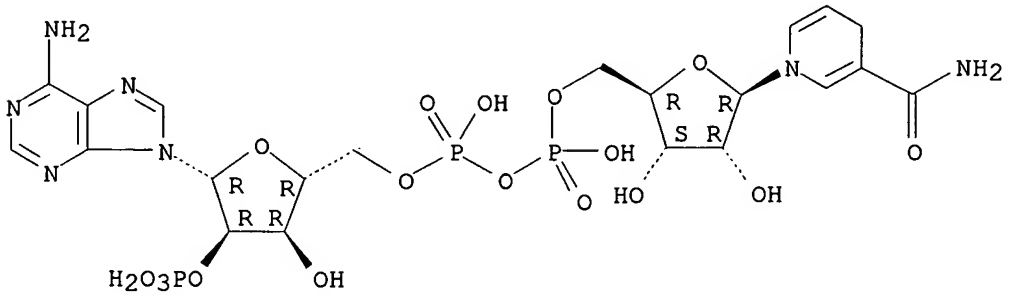
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

13781 REFERENCES IN FILE CA (1907 TO DATE)
269 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
13816 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L2 ANSWER 45 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **53-57-6** REGISTRY
ED Entered STN: 16 Nov 1984
CN Adenosine 5'-(trihydrogen diphosphate), 2'-(dihydrogen phosphate), P'→5'-ester with 1,4-dihydro-1-β-D-ribofuranosyl-3-pyridinecarboxamide (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Adenosine, 2'-(dihydrogen phosphate) 5'-(trihydrogen pyrophosphate), 5'→5'-ester with 1,4-dihydro-1-β-D-ribofuranosylnicotinamide (8CI)
OTHER NAMES:
CN β-NADPH
CN β-Nicotinamide-adenine-dinucleotide-phosphoric acid
CN β-TPNH
CN 51: PN: WO2004076659 FIGURE: 7 claimed sequence
CN Codehydrase II, reduced
CN Codehydrogenase II, reduced
CN Coenzyme II, reduced
CN Cozymase II, reduced
CN Dihydrocodehydrogenase II
CN NADPH
CN NADPH2
CN Nicotinamide-adenine dinucleotide phosphate, reduced
CN Reduced codehydrogenase II
CN Reduced nicotinamide adenine dinucleotide phosphate
CN Reduced triphosphopyridine nucleotide
CN TPNH
CN Triphosphopyridine nucleotide, reduced
FS STEREOSEARCH
DR 22046-90-8, 3545-01-5
MF C21 H30 N7 O17 P3

CI COM
LC STN Files: ADISNEWS, AGRICOLA, ANABSTR, BEILSTEIN*, BIOSIS, BIOTECHNO, CA, CABA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMLIST, CIN, CSCHEM, DDFU, DRUGU, EMBASE, IFICDB, IFIPAT, IFIUDB, IPA, MRCK*, PROMT, TOXCENTER, USPAT2, USPATFULL
(*File contains numerically searchable property data)
Other Sources: EINECS**, NDSL**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

11386 REFERENCES IN FILE CA (1907 TO DATE)
239 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
11421 REFERENCES IN FILE CAPLUS (1907 TO DATE)
57 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	86.82	89.52

FILE 'CAPLUS' ENTERED AT 14:32:35 ON 14 JUN 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 14 Jun 2006 VOL 144 ISS 25
FILE LAST UPDATED: 13 Jun 2006 (20060613/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/infopolicy.html

=> d his

(FILE 'HOME' ENTERED AT 14:30:32 ON 14 JUN 2006)

```
     FILE 'CAPLUS' ENTERED AT 14:30:42 ON 14 JUN 2006
L1             1 S US 20030086933/PN
                 SEL RN

     FILE 'REGISTRY' ENTERED AT 14:30:57 ON 14 JUN 2006
L2            45 S E1-E45

     FILE 'CAPLUS' ENTERED AT 14:32:35 ON 14 JUN 2006

=> s l2
L3         64271 L2

=> s prodrug (L) l3
           10858 PRODRUG
           10801 PRODRUGS
           15241 PRODRUG
                   (PRODRUG OR PRODRUGS)
L4           145 PRODRUG (L) L3

=>

=>
Executing the logoff script...


=> LOG H

COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     2.87      92.39

 SESSION WILL BE HELD FOR 60 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 14:33:52 ON 14 JUN 2006

Connecting via Winsock to STN



Welcome to STN International!  Enter x:x

LOGINID:SSSPTA1642BJF

PASSWORD:
 * * * * * * RECONNECTED TO STN INTERNATIONAL * * * * * *
SESSION RESUMED IN FILE 'CAPLUS' AT 14:39:43 ON 14 JUN 2006
FILE 'CAPLUS' ENTERED AT 14:39:43 ON 14 JUN 2006
COPYRIGHT (C) 2006 AMERICAN CHEMICAL SOCIETY (ACS)

COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     2.87      92.39

=> file caplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     3.33      92.85

FILE 'CAPLUS' ENTERED AT 14:40:17 ON 14 JUN 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2006 AMERICAN CHEMICAL SOCIETY (ACS)
```

FILE COVERS 1907 - 14 Jun 2006 VOL 144 ISS 25
FILE LAST UPDATED: 13 Jun 2006 (20060613/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/infopolicy.html

=> s 218443-93-7 or 218443-92-6 or 218443-91-5 or 218443-90-4 or 218443-88-0 or
126298-92-8 or 119643-82-2 or 115503-79-2 or 114554-11-9 or 109942-74-7 or
106047-77-2 or 99362-74-0 or 97009-81-9 or 89080-16-0 or 72306-81-1 or 64881-21-6
or 58880-44-7 or 52047-79-7 or 51652-08-5 or 212919-05-1
REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L6 4 L5

REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L8 12 L7

REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L10 3 L9

REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...

Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L12 4 L11

REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L14 5 L13

REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L16 3 L15

REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L18 5 L17

REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L20 13 L19

REG1stRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L22 4 L21

REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L24 3 L23

REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L26 2 L25

REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L28 2 L27

REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L30 2 L29

REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L32 2 L31

2 72306
149422 81
0 72306-81
(72306(W)81)
L33 33 L32 OR L30 OR L28 OR L26 OR L24 OR L22 OR L20 OR L18 OR L16 OR L14 OR L12 OR L10 OR L8 OR L6 OR 72306-81

=> s 17750-23-1 or 7145-37-1 or 6456-44-6 or 5463-59-2 or 4229-56-5 or 952-92-1 or 667919-86-0 or 218443-92-6 or 218443-91-5 or 218443-90-4 or 218443-88-0
REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L35 3 L34

REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L37 2 L36

REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L39 2 L38

REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L41 2 L40

REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L43 39 L42

REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L45 584 L44

REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L47 77 L46

REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L49 18 L48

REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L51 104 L50

REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L53 6 L52

REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L55 107 L54

L56 878 L55 OR L53 OR L51 OR L49 OR L47 OR L45 OR L43 OR L41 OR L39 OR L37 OR L35

```
=> file his
'HIS' IS NOT A VALID FILE NAME
SESSION CONTINUES IN FILE 'CAPLUS'
Enter "HELP FILE NAMES" at an arrow prompt (=>) for a list of files
that are available.  If you have requested multiple files, you can
specify a corrected file name or you can enter "IGNORE" to continue
accessing the remaining file names entered.

=> d his

     (FILE 'HOME' ENTERED AT 14:30:32 ON 14 JUN 2006)

     FILE 'CAPLUS' ENTERED AT 14:30:42 ON 14 JUN 2006
L1             1 S US 20030086933/PN
                 SEL RN

     FILE 'REGISTRY' ENTERED AT 14:30:57 ON 14 JUN 2006
L2            45 S E1-E45

     FILE 'CAPLUS' ENTERED AT 14:32:35 ON 14 JUN 2006
L3         64271 S L2
L4           145 S PRODRUG (L) L3

     FILE 'CAPLUS' ENTERED AT 14:40:17 ON 14 JUN 2006
                 S 218443-93-7/REG# OR  218443-92-6/REG# OR  218443-91-5/REG# OR

     FILE 'REGISTRY' ENTERED AT 14:43:18 ON 14 JUN 2006
L5             1 S 89080-16-0/RN

     FILE 'CAPLUS' ENTERED AT 14:43:18 ON 14 JUN 2006
L6             4 S L5

     FILE 'REGISTRY' ENTERED AT 14:43:19 ON 14 JUN 2006
L7             1 S 97009-81-9/RN

     FILE 'CAPLUS' ENTERED AT 14:43:19 ON 14 JUN 2006
L8            12 S L7

     FILE 'REGISTRY' ENTERED AT 14:43:20 ON 14 JUN 2006
L9             1 S 99362-74-0/RN

     FILE 'CAPLUS' ENTERED AT 14:43:20 ON 14 JUN 2006
L10            3 S L9

     FILE 'REGISTRY' ENTERED AT 14:43:21 ON 14 JUN 2006
L11            1 S 106047-77-2/RN

     FILE 'CAPLUS' ENTERED AT 14:43:21 ON 14 JUN 2006
L12            4 S L11

     FILE 'REGISTRY' ENTERED AT 14:43:22 ON 14 JUN 2006
L13            1 S 109942-74-7/RN

     FILE 'CAPLUS' ENTERED AT 14:43:22 ON 14 JUN 2006
L14            5 S L13

     FILE 'REGISTRY' ENTERED AT 14:43:23 ON 14 JUN 2006
L15            1 S 114554-11-9/RN
```

```
     FILE 'CAPLUS' ENTERED AT 14:43:23 ON 14 JUN 2006
L16           3 S L15

     FILE 'REGISTRY' ENTERED AT 14:43:24 ON 14 JUN 2006
L17           1 S 115503-79-2/RN

     FILE 'CAPLUS' ENTERED AT 14:43:24 ON 14 JUN 2006
L18           5 S L17

     FILE 'REGISTRY' ENTERED AT 14:43:25 ON 14 JUN 2006
L19           1 S 119643-82-2/RN

     FILE 'CAPLUS' ENTERED AT 14:43:25 ON 14 JUN 2006
L20          13 S L19

     FILE 'REGISTRY' ENTERED AT 14:43:26 ON 14 JUN 2006
L21           1 S 126298-92-8/RN

     FILE 'CAPLUS' ENTERED AT 14:43:26 ON 14 JUN 2006
L22           4 S L21

     FILE 'REGISTRY' ENTERED AT 14:43:27 ON 14 JUN 2006
L23           1 S 218443-88-0/RN

     FILE 'CAPLUS' ENTERED AT 14:43:28 ON 14 JUN 2006
L24           3 S L23

     FILE 'REGISTRY' ENTERED AT 14:43:28 ON 14 JUN 2006
L25           1 S 218443-90-4/RN

     FILE 'CAPLUS' ENTERED AT 14:43:29 ON 14 JUN 2006
L26           2 S L25

     FILE 'REGISTRY' ENTERED AT 14:43:29 ON 14 JUN 2006
L27           1 S 218443-91-5/RN

     FILE 'CAPLUS' ENTERED AT 14:43:30 ON 14 JUN 2006
L28           2 S L27

     FILE 'REGISTRY' ENTERED AT 14:43:30 ON 14 JUN 2006
L29           1 S 218443-92-6/RN

     FILE 'CAPLUS' ENTERED AT 14:43:31 ON 14 JUN 2006
L30           2 S L29

     FILE 'REGISTRY' ENTERED AT 14:43:31 ON 14 JUN 2006
L31           1 S 218443-93-7/RN

     FILE 'CAPLUS' ENTERED AT 14:43:32 ON 14 JUN 2006
L32           2 S L31
L33          33 S L32 OR L30 OR L28 OR L26 OR L24 OR L22 OR L20 OR L18 OR L16 O
                S 17750-23-1/REG# OR  7145-37-1/REG# OR  6456-44-6/REG# OR  546

     FILE 'REGISTRY' ENTERED AT 14:45:25 ON 14 JUN 2006
L34           1 S 218443-88-0/RN

     FILE 'CAPLUS' ENTERED AT 14:45:25 ON 14 JUN 2006
L35           3 S L34

     FILE 'REGISTRY' ENTERED AT 14:45:26 ON 14 JUN 2006
L36           1 S 218443-90-4/RN

     FILE 'CAPLUS' ENTERED AT 14:45:26 ON 14 JUN 2006
```

```
L37           2 S L36

     FILE 'REGISTRY' ENTERED AT 14:45:27 ON 14 JUN 2006
L38           1 S 218443-91-5/RN

     FILE 'CAPLUS' ENTERED AT 14:45:27 ON 14 JUN 2006
L39           2 S L38

     FILE 'REGISTRY' ENTERED AT 14:45:28 ON 14 JUN 2006
L40           1 S 218443-92-6/RN

     FILE 'CAPLUS' ENTERED AT 14:45:28 ON 14 JUN 2006
L41           2 S L40

     FILE 'REGISTRY' ENTERED AT 14:45:29 ON 14 JUN 2006
L42           1 S 667919-86-0/RN

     FILE 'CAPLUS' ENTERED AT 14:45:29 ON 14 JUN 2006
L43          39 S L42

     FILE 'REGISTRY' ENTERED AT 14:45:30 ON 14 JUN 2006
L44           1 S 952-92-1/RN

     FILE 'CAPLUS' ENTERED AT 14:45:30 ON 14 JUN 2006
L45         584 S L44

     FILE 'REGISTRY' ENTERED AT 14:45:31 ON 14 JUN 2006
L46           1 S 4229-56-5/RN

     FILE 'CAPLUS' ENTERED AT 14:45:32 ON 14 JUN 2006
L47          77 S L46

     FILE 'REGISTRY' ENTERED AT 14:45:32 ON 14 JUN 2006
L48           1 S 5463-59-2/RN

     FILE 'CAPLUS' ENTERED AT 14:45:32 ON 14 JUN 2006
L49          18 S L48

     FILE 'REGISTRY' ENTERED AT 14:45:33 ON 14 JUN 2006
L50           1 S 6456-44-6/RN

     FILE 'CAPLUS' ENTERED AT 14:45:33 ON 14 JUN 2006
L51         104 S L50

     FILE 'REGISTRY' ENTERED AT 14:45:34 ON 14 JUN 2006
L52           1 S 7145-37-1/RN

     FILE 'CAPLUS' ENTERED AT 14:45:34 ON 14 JUN 2006
L53           6 S L52

     FILE 'REGISTRY' ENTERED AT 14:45:35 ON 14 JUN 2006
L54           1 S 17750-23-1/RN

     FILE 'CAPLUS' ENTERED AT 14:45:35 ON 14 JUN 2006
L55         107 S L54
L56         878 S L55 OR L53 OR L51 OR L49 OR L47 OR L45 OR L43 OR L41 OR L39 O

=> s l33 or l56
L57        898 L33 OR L56

=> s CB (2W) 1954
          12521 CB
           3998 CBS
          16198 CB
```

```
                (CB OR CBS)
          8267 1954
L58         95 CB (2W) 1954

=> s CB (2W) 1954/cn
   REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.



PROXIMITY OPERATOR LEVEL NOT CONSISTENT WITH
FIELD CODE - 'AND' OPERATOR ASSUMED 'CB (2W) 1954/CN'


L60          0 L59

=> s cb1954
L61        104 CB1954

=> s cb-1954
          12521 CB
           3998 CBS
          16198 CB
                (CB OR CBS)
           8267 1954
L62         95 CB-1954
                (CB(W)1954)

=> s l62 or l61
L63        178 L62 OR L61

=> s l63 and l57
L64         18 L63 AND L57

=> s l64 not py>1997
       8391976 PY>1997
L65          9 L64 NOT PY>1997

=> s l64 not py>1996
       9151625 PY>1996
L66          7 L64 NOT PY>1996

=> d ibib 1-7

L66  ANSWER 1 OF 7  CAPLUS  COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER:         1994:203  CAPLUS
DOCUMENT NUMBER:          120:203
TITLE:                    Identification, synthesis and properties of
                          5-(aziridin-1-yl)-2-nitro-4-nitrosobenzamide, a novel
                          DNA crosslinking agent derived from CB1954
AUTHOR(S):                Knox, Richard J.; Friedlos, Frank; Biggs, Patrick J.;
                          Flitter, William D.; Gaskell, Margaret; Goddard,
                          Phyllis; Davies, Lawrence; Jarman, Michael
CORPORATE SOURCE:         Mol. Pharmacol. Unit, Inst. Cancer Res.,
                          Sutton/Surrey, SM2 5NG, UK
SOURCE:                   Biochemical Pharmacology (1993), 46(5), 797-803
                          CODEN: BCPCA6; ISSN: 0006-2952
DOCUMENT TYPE:            Journal
LANGUAGE:                 English

L66  ANSWER 2 OF 7  CAPLUS  COPYRIGHT 2006 ACS on STN
```

ACCESSION NUMBER: 1993:93913 CAPLUS
DOCUMENT NUMBER: 118:93913
TITLE: The bioactivation of 5-(aziridin-1-yl)-2,4-dinitrobenzamide (**CB1954**). II. A comparison of an Escherichia coli nitroreductase and Walker DT diaphorase
AUTHOR(S): Knox, Richard J.; Friedlos, Frank; Sherwood, Roger F.; Melton, Roger G.; Anlezark, Gillian M.
CORPORATE SOURCE: Mol. Pharmacol. Unit, Inst. Cancer Res., Sutton/Surrey, SM2 5NG, UK
SOURCE: Biochemical Pharmacology (1992), 44(12), 2297-301
CODEN: BCPCA6; ISSN: 0006-2952
DOCUMENT TYPE: Journal
LANGUAGE: English

L66 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1992:165847 CAPLUS
DOCUMENT NUMBER: 116:165847
TITLE: The differences in kinetics of rat and human DT diaphorase result in a differential sensitivity of derived cell lines to **CB 1954** (5-(aziridin-1-yl)-2,4-dinitrobenzamide) [Erratum to document cited in CA115(1):332c].
AUTHOR(S): Boland, Marion P.; Knox, Richard J.; Roberts, John J.
CORPORATE SOURCE: Mol. Pharmacol. Unit, Inst. Cancer Res., Sutton/Surrey, SM2 5NG, UK
SOURCE: Biochemical Pharmacology (1991), 42(Suppl.), S229
CODEN: BCPCA6; ISSN: 0006-2952
DOCUMENT TYPE: Journal
LANGUAGE: English

L66 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1992:34040 CAPLUS
DOCUMENT NUMBER: 116:34040
TITLE: Bioactivation of **CB 1954**: reaction of the active 4-hydroxylamino derivative with thioesters to form the ultimate DNA-DNA interstrand crosslinking species
AUTHOR(S): Knox, Richard J.; Friedlos, Frank; Marchbank, Tania; Roberts, John J.
CORPORATE SOURCE: Sect. Drug Dev., Inst. Cancer Res., Sutton/Surrey, SM2 5NG, UK
SOURCE: Biochemical Pharmacology (1991), 42(9), 1691-7
CODEN: BCPCA6; ISSN: 0006-2952
DOCUMENT TYPE: Journal
LANGUAGE: English

L66 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1991:421743 CAPLUS
DOCUMENT NUMBER: 115:21743
TITLE: Cytotoxicity and activation of **CB1954** in a human tumor cell line
AUTHOR(S): Sunters, Andrew; Baer, John; Bagshawe, Kenneth D.
CORPORATE SOURCE: Dep. Med. Oncol., Charing Cross Hosp., London, W6 8RF, UK
SOURCE: Biochemical Pharmacology (1991), 41(9), 1293-8
CODEN: BCPCA6; ISSN: 0006-2952
DOCUMENT TYPE: Journal
LANGUAGE: English

L66 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1991:400332 CAPLUS
DOCUMENT NUMBER: 115:332
TITLE: The differences in kinetics of rat and human DT

diaphorase result in a differential sensitivity of derived cell lines to **CB 1954** (5-(aziridin-1-yl)-2,4-dinitrobenzamide)

AUTHOR(S): Boland, Marion P.; Knox, Richard J.; Roberts, John J.

CORPORATE SOURCE: Mol. Pharmacol. Unit, Inst. Cancer Res., Sutton/Surrey, SM2 5NG, UK

SOURCE: Biochemical Pharmacology (1991), 41(6-7), 867-75
CODEN: BCPCA6; ISSN: 0006-2952

DOCUMENT TYPE: Journal

LANGUAGE: English

L66 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1989:128164 CAPLUS

DOCUMENT NUMBER: 110:128164

TITLE: A new cytotoxic, DNA interstrand crosslinking agent, 5-(aziridin-1-yl)-4-hydroxylamino-2-nitrobenzamide, is formed from 5-(aziridin-1-yl)-2,4-dinitrobenzamide (**CB 1954**) by a nitroreductase enzyme in Walker carcinoma cells

AUTHOR(S): Knox, Richard J.; Friedlos, Frank; Jarman, Michael; Roberts, John J.

CORPORATE SOURCE: Mol. Pharmacol. Unit, Inst. Cancer Res., Sutton/Surrey, SM2 5NG, UK

SOURCE: Biochemical Pharmacology (1988), 37(24), 4661-9
CODEN: BCPCA6; ISSN: 0006-2952

DOCUMENT TYPE: Journal

LANGUAGE: English

=> d kwic 5

L66 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN

TI Cytotoxicity and activation of **CB1954** in a human tumor cell line

AB **CB1954** (5-aziridin-1-yl-2,4-dinitrobenzamide) is a monofunctional alkylating agent, to which Walker 256 cells are very sensitive. These cells express a nitroreductase which reduces **CB1954** to a bifunctional crosslinking agent 5-(aziridin-1-yl)-4-hydroxylamino-2-nitrobenzamide. In vitro testing on the human colon line LS174T showed that the differential cytotoxicities between the monofunctional agent (**CB1954**), and the active species (generated in situ by the addition of NADH and the Walker rat nitroreductase) were smaller than anticipated due to the unexpected toxicity of **CB1954** (IC50 value for **CB1954** on LS174T cells of 78 μM). The toxicity of the chemical synthesized active form was less than if it had. . . an enzyme of similar mol. weight to that of the 33 kD Walker cell nitroreductase, which is capable of reducing **CB1954** to its toxic metabolite, and reducing MTT to its insol. formazan salt. The expression of this enzyme presumably accounts for the unexpected toxicity of **CB1954**.

ST **CB 1954** cytotoxicity activation colon tumor

IT Intestine, neoplasm
(colon, **CB1954** cytotoxicity and activation in)

IT 9037-41-6, Nitroreductase
RL: BIOL (Biological study)
(**CB1954** activation by, in human colon tumor cells)

IT 21919-05-1, **CB1954**
RL: PROC (Process)
(cytotoxicity and activation of, in human colon tumor cells)

IT **119643-82-2**
RL: PROC (Process)
(cytotoxicity and formation of, from **CB1954**, in human colon tumor cells)

```
=> FIL REGISTRY

COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                    21.96     216.79

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                    -0.75      -0.75

FILE 'REGISTRY' ENTERED AT 14:49:42 ON 14 JUN 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2006 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:   13 JUN 2006  HIGHEST RN 887650-39-7
DICTIONARY FILE UPDATES:  13 JUN 2006  HIGHEST RN 887650-39-7

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

**********************************************************************
*                                                                    *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added,   *
* effective March 20, 2005.  A new display format, IDERL, is now    *
* available and contains the CA role and document type information. *
*                                                                    *
**********************************************************************

Structure search iteration limits have been increased.  See HELP SLIMITS
for details.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=> S 119643-82-2/RN

L67          1 119643-82-2/RN

=> SET NOTICE 1 DISPLAY

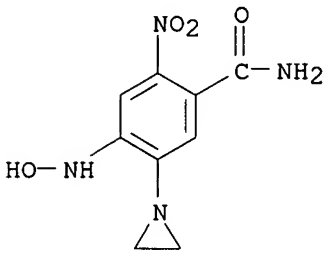
NOTICE SET TO 1 U.S. DOLLAR FOR DISPLAY COMMAND
SET COMMAND COMPLETED

=> D L67 SQIDE 1-

YOU HAVE REQUESTED DATA FROM 1 ANSWERS - CONTINUE? Y/(N):y
THE ESTIMATED COST FOR THIS REQUEST IS 6.36 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:y

L67  ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2006 ACS on STN
RN   119643-82-2  REGISTRY
```

CN Benzamide, 5-(1-aziridinyl)-4-(hydroxyamino)-2-nitro- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C9 H10 N4 O4
SR CA
LC STN Files: CA, CAPLUS, MEDLINE, TOXCENTER, USPATFULL
DT.CA CAplus document type: Journal; Patent
RL.P Roles from patents: BIOL (Biological study); FORM (Formation, nonpreparative); PREP (Preparation); USES (Uses)
RL.NP Roles from non-patents: BIOL (Biological study); FORM (Formation, nonpreparative); PREP (Preparation); PROC (Process); RACT (Reactant or reagent); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

13 REFERENCES IN FILE CA (1907 TO DATE)
13 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> SET NOTICE LOGIN DISPLAY

NOTICE SET TO OFF FOR DISPLAY COMMAND
SET COMMAND COMPLETED

=>

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	2.34	219.13

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-0.75

FILE 'CAPLUS' ENTERED AT 14:50:09 ON 14 JUN 2006

FILE COVERS 1907 - 14 Jun 2006 VOL 144 ISS 25
FILE LAST UPDATED: 13 Jun 2006 (20060613/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
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=> d l66 kwic 1-7

L66 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN
TI Identification, synthesis and properties of 5-(aziridin-1-yl)-2-nitro-4-nitrosobenzamide, a novel DNA crosslinking agent derived from **CB1954**
AB 5-(Aziridin-1-yl)-4-hydroxylamino-2-nitrobenzamide, the active form of the antitumor agent 5-(aziridin-1-yl)-2,4-dinitrobenzamide (**CB1954**), can react spontaneously with oxygen, and in aqueous solution yields 5-(aziridin-1-yl)-2-nitro-4-nitrosobenzamide and hydrogen peroxide. In order to understand fully the bioactivation of **CB1954**, chemical and biol. properties of the nitroso compound were studied. Mild biol. reducing agents such as NAD(P)H, reduced thiols, and. . . synthesis of 5-(aziridin-1-yl)-4-hydroxylamino-2-nitrobenzamide are described. These results emphasize the potential efficacy of the in situ activation of prodrugs such as **CB1954** either by endogenous enzymes such as DT diaphorase, or by antibody directed enzyme prodrug therapy (ADEPT).
ST antitumor aziridinyldinitrobenzamide bioactivation product cytotoxicity; DNA crosslinking antitumor **CB1954** bioactivation product; hydroxylaminobenzamide prepn cytotoxicity DNA crosslinking; nitrosobenzamide prepn cytotoxicity DNA crosslinking
IT Neoplasm inhibitors
(**CB1954** and its bioactivation products)
IT Deoxyribonucleic acids
RL: RCT (Reactant); RACT (Reactant or reagent)
(interstrand crosslinking of, by **CB1954** bioactivation products)
IT 21919-05-1, **CB1954**
RL: BIOL (Biological study)
(bioactivation products of, antitumor activity and cytotoxicity and DNA crosslinking by)
IT **119643-82-2P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and antitumor activity of, as **CB1954** active form)
IT 151602-22-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and antitumor activity of, as **CB1954** product)

L66 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN
TI The bioactivation of 5-(aziridin-1-yl)-2,4-dinitrobenzamide (**CB1954**). II. A comparison of an Escherichia coli nitroreductase and Walker DT diaphorase
AB A nitroreductase enzyme that has been isolated from Escherichia coli B is capable of bioactivating **CB1954** [5-(aziridin-1-yl)-2,4-dinitrobenzamide] to a cytotoxic agent, a property shared with the mammalian enzyme Walker DT diaphorase [NAD(P)H dehydrogenase (quinone), EC 1.6.99.2] as isolated from Walker cells. In contrast to Walker DT diaphorase, which can only reduce the 4-nitro group of **CB1954**, the E. coli nitroreductase can reduce either (but not both) nitro groups of **CB1954** to the corresponding hydroxylamino species. The two hydroxylamino species are formed in equal proportions and at the same rates. **CB1954** is reduced much more rapidly by the E. coli

nitroreductase than by Walker DT diaphorase. If the reduction of **CB1954** was carried out in the presence of V79 cells (which are insensitive to **CB1954**) a large cytotoxic effect was evident. This cytotoxicity was only observed under conditions in which the E. coli nitroreductase or. . . proposed that E. coli B nitroreductase would be a suitable enzyme for antibody-directed enzyme prodrug therapy (ADEPT) in combination with **CB1954**.

IT **119643-82-2** 119643-83-3
RL: FORM (Formation, nonpreparative)
(formation of, from aziridinyl dinitrobenzamide by nitroreductase of E. coli, antitumor activity in relation to)

L66 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN
TI The differences in kinetics of rat and human DT diaphorase result in a differential sensitivity of derived cell lines to **CB 1954** (5-(aziridin-1-yl)-2,4-dinitrobenzamide) [Erratum to document cited in CA115(1):332c].

IT **119643-82-2**
RL: FORM (Formation, nonpreparative)
(formation of, from **CB 1954**, DT diaphorase of humans and laboratory animals induction of (Erratum))

IT 9032-20-6
RL: PRP (Properties)
(kinetics of, of human and laboratory animal, differential sensitivity of tumors cells to **CB 1954** in relation to (Erratum))

L66 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN
TI Bioactivation of **CB 1954**: reaction of the active 4-hydroxylamino derivative with thioesters to form the ultimate DNA-DNA interstrand crosslinking species

AB 5-(Aziridin-1-yl)-4-hydroxylamino-2-nitrobenzamide (I) is the active form of **CB 1954** (5-(aziridin-1-yl)-2,4-dinitrobenzamide). This hydroxylamine is formed by the bioredn. of **CB 1954** by the enzyme DT diaphorase and accounts for the highly selective cytotoxicity of this compound The reason why the hydroxylamine derivative is so cytotoxic is that, in contrast to **CB 1954**, it can react difunctionally as characterized by the formation of DNA-DNA interstrand crosslinks in cells treated by this agent. However,. . . DNA reactive species was a minor product of the reaction. It is proposed that the ultimate, DNA reactive, derivative of **CB 1954** is 4-(N-acetoxy)-5-(aziridin-1-yl)-2-nitrobenzamide.

ST **CB 1954** bioactivation DNA crosslinking cytotoxicity

IT Neoplasm inhibitors
(**CB 1954** as, bioactivation in, DNA interstrand crosslinking in)

IT Deoxyribonucleic acids
RL: RCT (Reactant); RACT (Reactant or reagent)
(interstrand crosslinking of, by **CB 1954** bioactivation product, cytotoxicity in relation to)

IT Carboxylic acids, esters
RL: BIOL (Biological study)
(thio-, esters, **CB 1954** active metabolite binding to DNA response to, cytotoxicity in relation to)

IT 72-89-9, Acetyl coenzyme A 70019-69-1 70019-70-4
RL: BIOL (Biological study)
(**CB 1954** active metabolite binding to DNA response to, cytotoxicity in relation to)

IT 9032-20-6, DT Diaphorase
RL: BIOL (Biological study)
(**CB 1954** bioactivation by, DNA interstrand crosslinking from, thioesters in, cytotoxicity in relation to)

IT 21919-05-1, **CB 1954**
RL: BIOL (Biological study)

(bioactivation of, DNA-DNA interstrand crosslinking in, thioesters in)
IT 1866-15-5, S-Acetylthiocholine iodide
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with **CB 1954** active metabolite, DNA crosslinking in, cytotoxicity in relation to)
IT **119643-82-2**
RL: BIOL (Biological study)
(reaction with DNA of, as **CB 1954** metabolite, thioesters effect on, cytotoxicity in relation to)

L66 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN
TI Cytotoxicity and activation of **CB1954** in a human tumor cell line
AB **CB1954** (5-aziridin-1-yl-2,4-dinitrobenzamide) is a monofunctional alkylating agent, to which Walker 256 cells are very sensitive. These cells express a nitroreductase which reduces **CB1954** to a bifunctional crosslinking agent 5-(aziridin-1-yl)-4-hydroxylamino-2-nitrobenzamide. In vitro testing on the human colon line LS174T showed that the differential cytotoxicities between the monofunctional agent (**CB1954**), and the active species (generated in situ by the addition of NADH and the Walker rat nitroreductase) were smaller than anticipated due to the unexpected toxicity of **CB1954** (IC50 value for **CB1954** on LS174T cells of 78 μM). The toxicity of the chemical synthesized active form was less than if it had. . . an enzyme of similar mol. weight to that of the 33 kD Walker cell nitroreductase, which is capable of reducing **CB1954** to its toxic metabolite, and reducing MTT to its insol. formazan salt. The expression of this enzyme presumably accounts for the unexpected toxicity of **CB1954**.
ST **CB 1954** cytotoxicity activation colon tumor
IT Intestine, neoplasm
(colon, **CB1954** cytotoxicity and activation in)
IT 9037-41-6, Nitroreductase
RL: BIOL (Biological study)
(**CB1954** activation by, in human colon tumor cells)
IT 21919-05-1, **CB1954**
RL: PROC (Process)
(cytotoxicity and activation of, in human colon tumor cells)
IT **119643-82-2**
RL: PROC (Process)
(cytotoxicity and formation of, from **CB1954**, in human colon tumor cells)

L66 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN
TI The differences in kinetics of rat and human DT diaphorase result in a differential sensitivity of derived cell lines to **CB 1954** (5-(aziridin-1-yl)-2,4-dinitrobenzamide)
AB DT diaphorase (NAD(P)H dehydrogenase (quinone), EC 1.6.99.2) isolated from Walker 256 rat carcinoma cells can convert **CB 1954** to a cytotoxic DNA interstrand crosslinking agent. This is achieved by reduction of the 4-nitro group of **CB 1954** to produce the hydroxylamino species, a bioactivation which accounts for the much greater sensitivity of Walker cells to **CB 1954** when compared with other cells which are unable to carry out this reduction As predicted from their measured DT diaphorase activities a number of rat hepatoma and hepatocyte cell lines were also shown to be sensitive to **CB 1954**. However, no **CB 1954**-sensitive cell lines of human origin were found, although levels of DT diaphorase similar to those in the sensitive rat cells were present in these cells. The human cells were as sensitive as rat cells to the active form of **CB 1954** (5-(aziridin-1-yl)-4-hydroxylamino-2-nitrobenzamide). DT diaphorase, purified to homogeneity from human Hep G2 cells, did metabolize **CB 1954** to this 4-hydroxylamino product, but the rate of **CB 1954** reduction and thus production of the cytotoxic product, was much lower than that of purified Walker

enzyme (ratio of Kcat = 6.4). In addition, **CB 1954** could be considered an inhibitor of, rather than a substrate for, the human form of DT diaphorase. The purified rat and human DT diaphorases possessed otherwise similar biochem. and mol. properties. These findings explain the decreased sensitivity towards **CB 1954** of human cell lines when compared to rat cell lines.

IT **119643-82-2**
RL: FORM (Formation, nonpreparative)
(formation of, from **CB 1954**, DT diaphorase of humans and laboratory animals induction of)

IT 9032-20-6
RL: PRP (Properties)
(kinetics of, of human and laboratory animal, differential sensitivity of tumors cells to **CB 1954** in relation to)

IT 21919-05-1, **CB 1954**
RL: BIOL (Biological study)
(tumor sensitivity to, of humans and laboratory animals, DT diaphorase kinetics in relation to)

L66 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN

TI A new cytotoxic, DNA interstrand crosslinking agent, 5-(aziridin-1-yl)-4-hydroxylamino-2-nitrobenzamide, is formed from 5-(aziridin-1-yl)-2,4-dinitrobenzamide (**CB 1954**) by a nitroreductase enzyme in Walker carcinoma cells

AB Walker tumor cells in vivo or in vitro are exceptionally sensitive to the monofunctional alkylating agent **CB 1954**. **CB 1954** forms DNA interstrand crosslinks in a time-dependent manner in Walker tumor cells but not in nontoxically affected Chinese hamster V79 cells. However, coculturing Chinese hamster V79 cells with Walker cells in the presence of **CB 1954** rendered the hamster cells sensitive to **CB 1954** and led to the formation of interstrand crosslinks in their DNA, findings indicative of the formation by Walker cells of a diffusible toxic metabolite of **CB 1954**. A flavoprotein, of mol. weight 33.5 kDa as estimated by SDS-polyacrylamide gel electrophoresis, was isolated from Walker cells and identified. . . dehydrogenase (quinone) (DT diaphorase, EC 1.6.99.2). This enzyme, in the presence of NADH or NADPH, catalyzed the aerobic reduction of **CB 1954** to 5-(aziridin-1-yl)-4-hydroxylamino-2-nitrobenzamide. This new compound can form interstrand crosslinks in the DNA of Chinese hamster V79 cells to which it. . .

ST **CB 1954** antitumor NADPH dehydrogenase prepn

IT Deoxyribonucleic acids
RL: RCT (Reactant); RACT (Reactant or reagent)
(crosslinking of, by **CB 1954**, metabolism by NADPH dehydrogenase in)

IT Neoplasm inhibitors
(carcinoma, **CB 1954** as, metabolism by NADPH dehydrogenase in)

IT 9032-20-6, NAD(P)H dehydrogenase
RL: BIOL (Biological study)
(**CB 1954** metabolism to antitumor metabolite by)

IT **119643-82-2**
RL: FORM (Formation, nonpreparative)
(formation of, as **CB 1954** antitumor metabolite)

IT 21919-05-1, **CB 1954**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(neoplasm inhibition by, DNA crosslinking by metabolite in)

IT 61837-23-8P 61837-26-1P 119643-83-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and formation as **CB 1954** metabolite of, neoplasm inhibition in relation to)

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=> FIL REGISTRY

COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                    13.29     232.42

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
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CA SUBSCRIBER PRICE                                    -4.50      -5.25

FILE 'REGISTRY' ENTERED AT 14:51:48 ON 14 JUN 2006
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STRUCTURE FILE UPDATES:   13 JUN 2006  HIGHEST RN 887650-39-7
DICTIONARY FILE UPDATES:  13 JUN 2006  HIGHEST RN 887650-39-7

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TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

  Please note that search-term pricing does apply when
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**********************************************************************
*                                                                    *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added,   *
* effective March 20, 2005.  A new display format, IDERL, is now    *
* available and contains the CA role and document type information. *
*                                                                    *
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Structure search iteration limits have been increased.  See HELP SLIMITS
for details.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=> S 119643-83-3/RN

L68          1 119643-83-3/RN

=> SET NOTICE 1 DISPLAY

NOTICE SET TO 1 U.S. DOLLAR FOR DISPLAY COMMAND
SET COMMAND COMPLETED

=> D L68 SQIDE 1-

YOU HAVE REQUESTED DATA FROM 1 ANSWERS - CONTINUE? Y/(N):y
THE ESTIMATED COST FOR THIS REQUEST IS 6.36 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:y

L68  ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2006 ACS on STN
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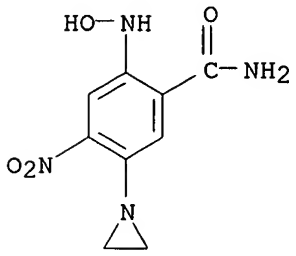
RN **119643-83-3** REGISTRY
CN Benzamide, 5-(1-aziridinyl)-2-(hydroxyamino)-4-nitro- (9CI) (CA INDEX NAME)
MF C9 H10 N4 O4
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: BIOL (Biological study); FORM (Formation, nonpreparative); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

6 REFERENCES IN FILE CA (1907 TO DATE)
6 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> SET NOTICE LOGIN DISPLAY

NOTICE SET TO OFF FOR DISPLAY COMMAND
SET COMMAND COMPLETED

=>

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	2.34	234.76

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-5.25

FILE 'CAPLUS' ENTERED AT 14:52:04 ON 14 JUN 2006

FILE COVERS 1907 - 14 Jun 2006 VOL 144 ISS 25
FILE LAST UPDATED: 13 Jun 2006 (20060613/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
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=> d his

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                 SEL RN

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L2            45 S E1-E45

     FILE 'CAPLUS' ENTERED AT 14:32:35 ON 14 JUN 2006
L3         64271 S L2
L4           145 S PRODRUG (L) L3

     FILE 'CAPLUS' ENTERED AT 14:40:17 ON 14 JUN 2006
                 S 218443-93-7/REG# OR  218443-92-6/REG# OR  218443-91-5/REG# OR

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L5             1 S 89080-16-0/RN

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L6             4 S L5

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L19           1 S 119643-82-2/RN

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L20          13 S L19

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L22           4 S L21

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L23           1 S 218443-88-0/RN

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L24           3 S L23

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L25           1 S 218443-90-4/RN

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L26           2 S L25

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L27           1 S 218443-91-5/RN

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L29           1 S 218443-92-6/RN

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L30           2 S L29

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L31           1 S 218443-93-7/RN

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L37           2 S L36

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L38           1 S 218443-91-5/RN

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L39           2 S L38
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L44           1 S 952-92-1/RN

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L46           1 S 4229-56-5/RN

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L47          77 S L46

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L48           1 S 5463-59-2/RN

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L52           1 S 7145-37-1/RN

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L53           6 S L52

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L54           1 S 17750-23-1/RN

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L56         878 S L55 OR L53 OR L51 OR L49 OR L47 OR L45 OR L43 OR L41 OR L39 O
L57         898 S L33 OR L56
L58          95 S CB (2W) 1954
                S CB (2W) 1954/CN

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L61         104 S CB1954
L62          95 S CB-1954
L63         178 S L62 OR L61
L64          18 S L63 AND L57
L65           9 S L64 NOT PY>1997
L66           7 S L64 NOT PY>1996
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                 SET NOTICE LOGIN DISPLAY

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     FILE 'REGISTRY' ENTERED AT 14:51:48 ON 14 JUN 2006
L68            1 S 119643-83-3/RN
                 SET NOTICE 1 DISPLAY
                 SET NOTICE LOGIN DISPLAY

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=> d his

     (FILE 'HOME' ENTERED AT 14:30:32 ON 14 JUN 2006)

     FILE 'CAPLUS' ENTERED AT 14:30:42 ON 14 JUN 2006
L1             1 S US 20030086933/PN
                 SEL RN

     FILE 'REGISTRY' ENTERED AT 14:30:57 ON 14 JUN 2006
L2            45 S E1-E45

     FILE 'CAPLUS' ENTERED AT 14:32:35 ON 14 JUN 2006
L3         64271 S L2
L4           145 S PRODRUG (L) L3

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L5             1 S 89080-16-0/RN

     FILE 'CAPLUS' ENTERED AT 14:43:18 ON 14 JUN 2006
L6             4 S L5

     FILE 'REGISTRY' ENTERED AT 14:43:19 ON 14 JUN 2006
L7             1 S 97009-81-9/RN

     FILE 'CAPLUS' ENTERED AT 14:43:19 ON 14 JUN 2006
L8            12 S L7

     FILE 'REGISTRY' ENTERED AT 14:43:20 ON 14 JUN 2006
L9             1 S 99362-74-0/RN

     FILE 'CAPLUS' ENTERED AT 14:43:20 ON 14 JUN 2006
L10            3 S L9

     FILE 'REGISTRY' ENTERED AT 14:43:21 ON 14 JUN 2006
L11            1 S 106047-77-2/RN

     FILE 'CAPLUS' ENTERED AT 14:43:21 ON 14 JUN 2006
L12            4 S L11

     FILE 'REGISTRY' ENTERED AT 14:43:22 ON 14 JUN 2006
L13            1 S 109942-74-7/RN

     FILE 'CAPLUS' ENTERED AT 14:43:22 ON 14 JUN 2006
L14            5 S L13

     FILE 'REGISTRY' ENTERED AT 14:43:23 ON 14 JUN 2006
L15            1 S 114554-11-9/RN
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     FILE 'CAPLUS' ENTERED AT 14:43:23 ON 14 JUN 2006
L16           3 S L15

     FILE 'REGISTRY' ENTERED AT 14:43:24 ON 14 JUN 2006
L17           1 S 115503-79-2/RN

     FILE 'CAPLUS' ENTERED AT 14:43:24 ON 14 JUN 2006
L18           5 S L17

     FILE 'REGISTRY' ENTERED AT 14:43:25 ON 14 JUN 2006
L19           1 S 119643-82-2/RN

     FILE 'CAPLUS' ENTERED AT 14:43:25 ON 14 JUN 2006
L20          13 S L19

     FILE 'REGISTRY' ENTERED AT 14:43:26 ON 14 JUN 2006
L21           1 S 126298-92-8/RN

     FILE 'CAPLUS' ENTERED AT 14:43:26 ON 14 JUN 2006
L22           4 S L21

     FILE 'REGISTRY' ENTERED AT 14:43:27 ON 14 JUN 2006
L23           1 S 218443-88-0/RN

     FILE 'CAPLUS' ENTERED AT 14:43:28 ON 14 JUN 2006
L24           3 S L23

     FILE 'REGISTRY' ENTERED AT 14:43:28 ON 14 JUN 2006
L25           1 S 218443-90-4/RN

     FILE 'CAPLUS' ENTERED AT 14:43:29 ON 14 JUN 2006
L26           2 S L25

     FILE 'REGISTRY' ENTERED AT 14:43:29 ON 14 JUN 2006
L27           1 S 218443-91-5/RN

     FILE 'CAPLUS' ENTERED AT 14:43:30 ON 14 JUN 2006
L28           2 S L27

     FILE 'REGISTRY' ENTERED AT 14:43:30 ON 14 JUN 2006
L29           1 S 218443-92-6/RN

     FILE 'CAPLUS' ENTERED AT 14:43:31 ON 14 JUN 2006
L30           2 S L29

     FILE 'REGISTRY' ENTERED AT 14:43:31 ON 14 JUN 2006
L31           1 S 218443-93-7/RN

     FILE 'CAPLUS' ENTERED AT 14:43:32 ON 14 JUN 2006
L32           2 S L31
L33          33 S L32 OR L30 OR L28 OR L26 OR L24 OR L22 OR L20 OR L18 OR L16 O
                S 17750-23-1/REG# OR  7145-37-1/REG# OR  6456-44-6/REG# OR  546

     FILE 'REGISTRY' ENTERED AT 14:45:25 ON 14 JUN 2006
L34           1 S 218443-88-0/RN

     FILE 'CAPLUS' ENTERED AT 14:45:25 ON 14 JUN 2006
L35           3 S L34

     FILE 'REGISTRY' ENTERED AT 14:45:26 ON 14 JUN 2006
L36           1 S 218443-90-4/RN

     FILE 'CAPLUS' ENTERED AT 14:45:26 ON 14 JUN 2006
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L37           2 S L36

     FILE 'REGISTRY' ENTERED AT 14:45:27 ON 14 JUN 2006
L38           1 S 218443-91-5/RN

     FILE 'CAPLUS' ENTERED AT 14:45:27 ON 14 JUN 2006
L39           2 S L38

     FILE 'REGISTRY' ENTERED AT 14:45:28 ON 14 JUN 2006
L40           1 S 218443-92-6/RN

     FILE 'CAPLUS' ENTERED AT 14:45:28 ON 14 JUN 2006
L41           2 S L40

     FILE 'REGISTRY' ENTERED AT 14:45:29 ON 14 JUN 2006
L42           1 S 667919-86-0/RN

     FILE 'CAPLUS' ENTERED AT 14:45:29 ON 14 JUN 2006
L43          39 S L42

     FILE 'REGISTRY' ENTERED AT 14:45:30 ON 14 JUN 2006
L44           1 S 952-92-1/RN

     FILE 'CAPLUS' ENTERED AT 14:45:30 ON 14 JUN 2006
L45         584 S L44

     FILE 'REGISTRY' ENTERED AT 14:45:31 ON 14 JUN 2006
L46           1 S 4229-56-5/RN

     FILE 'CAPLUS' ENTERED AT 14:45:32 ON 14 JUN 2006
L47          77 S L46

     FILE 'REGISTRY' ENTERED AT 14:45:32 ON 14 JUN 2006
L48           1 S 5463-59-2/RN

     FILE 'CAPLUS' ENTERED AT 14:45:32 ON 14 JUN 2006
L49          18 S L48

     FILE 'REGISTRY' ENTERED AT 14:45:33 ON 14 JUN 2006
L50           1 S 6456-44-6/RN

     FILE 'CAPLUS' ENTERED AT 14:45:33 ON 14 JUN 2006
L51         104 S L50

     FILE 'REGISTRY' ENTERED AT 14:45:34 ON 14 JUN 2006
L52           1 S 7145-37-1/RN

     FILE 'CAPLUS' ENTERED AT 14:45:34 ON 14 JUN 2006
L53           6 S L52

     FILE 'REGISTRY' ENTERED AT 14:45:35 ON 14 JUN 2006
L54           1 S 17750-23-1/RN

     FILE 'CAPLUS' ENTERED AT 14:45:35 ON 14 JUN 2006
L55         107 S L54
L56         878 S L55 OR L53 OR L51 OR L49 OR L47 OR L45 OR L43 OR L41 OR L39 O
L57         898 S L33 OR L56
L58          95 S CB (2W) 1954
                S CB (2W) 1954/CN

     FILE 'REGISTRY' ENTERED AT 14:46:25 ON 14 JUN 2006
L59           0 S CB (2W) 1954/CN

     FILE 'CAPLUS' ENTERED AT 14:46:25 ON 14 JUN 2006
```

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L60           0 S L59
L61         104 S CB1954
L62          95 S CB-1954
L63         178 S L62 OR L61
L64          18 S L63 AND L57
L65           9 S L64 NOT PY>1997
L66           7 S L64 NOT PY>1996

     FILE 'REGISTRY' ENTERED AT 14:49:42 ON 14 JUN 2006
L67           1 S 119643-82-2/RN
                SET NOTICE 1 DISPLAY
                SET NOTICE LOGIN DISPLAY

     FILE 'CAPLUS' ENTERED AT 14:50:09 ON 14 JUN 2006

     FILE 'REGISTRY' ENTERED AT 14:51:48 ON 14 JUN 2006
L68           1 S 119643-83-3/RN
                SET NOTICE 1 DISPLAY
                SET NOTICE LOGIN DISPLAY

     FILE 'CAPLUS' ENTERED AT 14:52:04 ON 14 JUN 2006

=> s l57 not 119643-82-2
   REGISTRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.




L70          13 L69


L71         885 L57 NOT L70


=> s l71 and prodrug
          10858 PRODRUG
          10801 PRODRUGS
          15241 PRODRUG
                  (PRODRUG OR PRODRUGS)
L72           6 L71 AND PRODRUG

=> d ibib 1-6

L72  ANSWER 1 OF 6  CAPLUS  COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER:         2004:301733  CAPLUS
DOCUMENT NUMBER:          141:306746
TITLE:                    Quinone reductase-mediated nitro-reduction: clinical
                          applications
AUTHOR(S):                Knox, Richard J.; Chen, Shiuan
CORPORATE SOURCE:         Enact Pharma PLC, Salisbury, SP4 0JQ, UK
SOURCE:                   Methods in Enzymology (2004), 382(Quinones and Quinone
                          Enzymes, Part B), 194-221
                          CODEN: MENZAU; ISSN: 0076-6879
PUBLISHER:                Elsevier
DOCUMENT TYPE:            Journal; General Review
LANGUAGE:                 English
REFERENCE COUNT:          92    THERE ARE 92 CITED REFERENCES AVAILABLE FOR THIS
                                RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
```

L72 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:749515 CAPLUS
DOCUMENT NUMBER: 140:121861
TITLE: CB 1954: From the Walker tumor to NQO2 and VDEPT
AUTHOR(S): Knox, Richard J.; Burke, Philip J.; Chen, Shiuan; Kerr, David J.
CORPORATE SOURCE: Enact Pharma PLC, Salisbury, UK
SOURCE: Current Pharmaceutical Design (2003), 9(26), 2091-2104
CODEN: CPDEFP; ISSN: 1381-6128
PUBLISHER: Bentham Science Publishers Ltd.
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
REFERENCE COUNT: 97 THERE ARE 97 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L72 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:835107 CAPLUS
DOCUMENT NUMBER: 139:414
TITLE: Improved cancer treatment with enzyme technology
CORPORATE SOURCE: Enact Pharma, Enact Pharma plc, Salisbury, SP4 0JQ, UK
SOURCE: sp2 (2002), 1(8), 22, 24-25
CODEN: SPSUCF; ISSN: 1476-184X
PUBLISHER: Avakado Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

L72 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:584913 CAPLUS
DOCUMENT NUMBER: 135:338611
TITLE: Aerobic nitroreduction by flavoproteins: enzyme structure, mechanisms and role in cancer chemotherapy
AUTHOR(S): Skelly, Jane V.; Knox, Richard J.; Jenkins, Terence C.
CORPORATE SOURCE: School of Chemical and Life Sciences, University of Greenwich, London, SE18 6PF, UK
SOURCE: Mini-Reviews in Medicinal Chemistry (2001), 1(3), 293-306
CODEN: MMCIAE; ISSN: 1389-5575
PUBLISHER: Bentham Science Publishers Ltd.
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
REFERENCE COUNT: 97 THERE ARE 97 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L72 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:597759 CAPLUS
DOCUMENT NUMBER: 133:275962
TITLE: Bioactivation of 5-(aziridin-1-yl)-2,4-dinitrobenzamide (CB 1954) by human NAD(P)H quinone oxidoreductase 2: a novel co-substrate-mediated antitumor **prodrug** therapy
AUTHOR(S): Knox, Richard J.; Jenkins, Terence C.; Hobbs, Stephen M.; Chen, Shiuan; Melton, Roger G.; Burke, Philip J.
CORPORATE SOURCE: Enact Pharma Plc, Salisbury, SP4 0JQ, UK
SOURCE: Cancer Research (2000), 60(15), 4179-4186
CODEN: CNREA8; ISSN: 0008-5472
PUBLISHER: American Association for Cancer Research
DOCUMENT TYPE: Journal
LANGUAGE: English
REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L72 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:124026 CAPLUS
DOCUMENT NUMBER: 130:306493

TITLE: Formation of N-methylnicotinamide in the brain from a dihydropyridine-type **prodrug**: effect on brain choline
AUTHOR(S): Erb, Christina; Seidel, Albrecht; Frank, Heinz; Platt, Karl L.; Oesch, Franz; Klein, Jochen
CORPORATE SOURCE: Department of Pharmacology, University of Mainz, Mainz, D'55101, Germany
SOURCE: Biochemical Pharmacology (1999), 57(6), 681-684
CODEN: BCPCA6; ISSN: 0006-2952
PUBLISHER: Elsevier Science Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> s 21919-05-1
REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L74 176 L73

=> d his

(FILE 'HOME' ENTERED AT 14:30:32 ON 14 JUN 2006)

FILE 'CAPLUS' ENTERED AT 14:30:42 ON 14 JUN 2006
L1 1 S US 20030086933/PN
SEL RN

FILE 'REGISTRY' ENTERED AT 14:30:57 ON 14 JUN 2006
L2 45 S E1-E45

FILE 'CAPLUS' ENTERED AT 14:32:35 ON 14 JUN 2006
L3 64271 S L2
L4 145 S PRODRUG (L) L3

FILE 'CAPLUS' ENTERED AT 14:40:17 ON 14 JUN 2006
S 218443-93-7/REG# OR 218443-92-6/REG# OR 218443-91-5/REG# OR

FILE 'REGISTRY' ENTERED AT 14:43:18 ON 14 JUN 2006
L5 1 S 89080-16-0/RN

FILE 'CAPLUS' ENTERED AT 14:43:18 ON 14 JUN 2006
L6 4 S L5

FILE 'REGISTRY' ENTERED AT 14:43:19 ON 14 JUN 2006
L7 1 S 97009-81-9/RN

FILE 'CAPLUS' ENTERED AT 14:43:19 ON 14 JUN 2006
L8 12 S L7

FILE 'REGISTRY' ENTERED AT 14:43:20 ON 14 JUN 2006
L9 1 S 99362-74-0/RN

FILE 'CAPLUS' ENTERED AT 14:43:20 ON 14 JUN 2006

```
L10           3 S L9

     FILE 'REGISTRY' ENTERED AT 14:43:21 ON 14 JUN 2006
L11           1 S 106047-77-2/RN

     FILE 'CAPLUS' ENTERED AT 14:43:21 ON 14 JUN 2006
L12           4 S L11

     FILE 'REGISTRY' ENTERED AT 14:43:22 ON 14 JUN 2006
L13           1 S 109942-74-7/RN

     FILE 'CAPLUS' ENTERED AT 14:43:22 ON 14 JUN 2006
L14           5 S L13

     FILE 'REGISTRY' ENTERED AT 14:43:23 ON 14 JUN 2006
L15           1 S 114554-11-9/RN

     FILE 'CAPLUS' ENTERED AT 14:43:23 ON 14 JUN 2006
L16           3 S L15

     FILE 'REGISTRY' ENTERED AT 14:43:24 ON 14 JUN 2006
L17           1 S 115503-79-2/RN

     FILE 'CAPLUS' ENTERED AT 14:43:24 ON 14 JUN 2006
L18           5 S L17

     FILE 'REGISTRY' ENTERED AT 14:43:25 ON 14 JUN 2006
L19           1 S 119643-82-2/RN

     FILE 'CAPLUS' ENTERED AT 14:43:25 ON 14 JUN 2006
L20          13 S L19

     FILE 'REGISTRY' ENTERED AT 14:43:26 ON 14 JUN 2006
L21           1 S 126298-92-8/RN

     FILE 'CAPLUS' ENTERED AT 14:43:26 ON 14 JUN 2006
L22           4 S L21

     FILE 'REGISTRY' ENTERED AT 14:43:27 ON 14 JUN 2006
L23           1 S 218443-88-0/RN

     FILE 'CAPLUS' ENTERED AT 14:43:28 ON 14 JUN 2006
L24           3 S L23

     FILE 'REGISTRY' ENTERED AT 14:43:28 ON 14 JUN 2006
L25           1 S 218443-90-4/RN

     FILE 'CAPLUS' ENTERED AT 14:43:29 ON 14 JUN 2006
L26           2 S L25

     FILE 'REGISTRY' ENTERED AT 14:43:29 ON 14 JUN 2006
L27           1 S 218443-91-5/RN

     FILE 'CAPLUS' ENTERED AT 14:43:30 ON 14 JUN 2006
L28           2 S L27

     FILE 'REGISTRY' ENTERED AT 14:43:30 ON 14 JUN 2006
L29           1 S 218443-92-6/RN

     FILE 'CAPLUS' ENTERED AT 14:43:31 ON 14 JUN 2006
L30           2 S L29

     FILE 'REGISTRY' ENTERED AT 14:43:31 ON 14 JUN 2006
L31           1 S 218443-93-7/RN
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     FILE 'CAPLUS' ENTERED AT 14:43:32 ON 14 JUN 2006
L32            2 S L31
L33           33 S L32 OR L30 OR L28 OR L26 OR L24 OR L22 OR L20 OR L18 OR L16 O
                  S 17750-23-1/REG# OR  7145-37-1/REG# OR  6456-44-6/REG# OR  546

     FILE 'REGISTRY' ENTERED AT 14:45:25 ON 14 JUN 2006
L34            1 S 218443-88-0/RN

     FILE 'CAPLUS' ENTERED AT 14:45:25 ON 14 JUN 2006
L35            3 S L34

     FILE 'REGISTRY' ENTERED AT 14:45:26 ON 14 JUN 2006
L36            1 S 218443-90-4/RN

     FILE 'CAPLUS' ENTERED AT 14:45:26 ON 14 JUN 2006
L37            2 S L36

     FILE 'REGISTRY' ENTERED AT 14:45:27 ON 14 JUN 2006
L38            1 S 218443-91-5/RN

     FILE 'CAPLUS' ENTERED AT 14:45:27 ON 14 JUN 2006
L39            2 S L38

     FILE 'REGISTRY' ENTERED AT 14:45:28 ON 14 JUN 2006
L40            1 S 218443-92-6/RN

     FILE 'CAPLUS' ENTERED AT 14:45:28 ON 14 JUN 2006
L41            2 S L40

     FILE 'REGISTRY' ENTERED AT 14:45:29 ON 14 JUN 2006
L42            1 S 667919-86-0/RN

     FILE 'CAPLUS' ENTERED AT 14:45:29 ON 14 JUN 2006
L43           39 S L42

     FILE 'REGISTRY' ENTERED AT 14:45:30 ON 14 JUN 2006
L44            1 S 952-92-1/RN

     FILE 'CAPLUS' ENTERED AT 14:45:30 ON 14 JUN 2006
L45          584 S L44

     FILE 'REGISTRY' ENTERED AT 14:45:31 ON 14 JUN 2006
L46            1 S 4229-56-5/RN

     FILE 'CAPLUS' ENTERED AT 14:45:32 ON 14 JUN 2006
L47           77 S L46

     FILE 'REGISTRY' ENTERED AT 14:45:32 ON 14 JUN 2006
L48            1 S 5463-59-2/RN

     FILE 'CAPLUS' ENTERED AT 14:45:32 ON 14 JUN 2006
L49           18 S L48

     FILE 'REGISTRY' ENTERED AT 14:45:33 ON 14 JUN 2006
L50            1 S 6456-44-6/RN

     FILE 'CAPLUS' ENTERED AT 14:45:33 ON 14 JUN 2006
L51          104 S L50

     FILE 'REGISTRY' ENTERED AT 14:45:34 ON 14 JUN 2006
L52            1 S 7145-37-1/RN

     FILE 'CAPLUS' ENTERED AT 14:45:34 ON 14 JUN 2006
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L53             6 S L52

     FILE 'REGISTRY' ENTERED AT 14:45:35 ON 14 JUN 2006
L54             1 S 17750-23-1/RN

     FILE 'CAPLUS' ENTERED AT 14:45:35 ON 14 JUN 2006
L55           107 S L54
L56           878 S L55 OR L53 OR L51 OR L49 OR L47 OR L45 OR L43 OR L41 OR L39 O
L57           898 S L33 OR L56
L58            95 S CB (2W) 1954
                  S CB (2W) 1954/CN

     FILE 'REGISTRY' ENTERED AT 14:46:25 ON 14 JUN 2006
L59             0 S CB (2W) 1954/CN

     FILE 'CAPLUS' ENTERED AT 14:46:25 ON 14 JUN 2006
L60             0 S L59
L61           104 S CB1954
L62            95 S CB-1954
L63           178 S L62 OR L61
L64            18 S L63 AND L57
L65             9 S L64 NOT PY>1997
L66             7 S L64 NOT PY>1996

     FILE 'REGISTRY' ENTERED AT 14:49:42 ON 14 JUN 2006
L67             1 S 119643-82-2/RN
                  SET NOTICE 1 DISPLAY
                  SET NOTICE LOGIN DISPLAY

     FILE 'CAPLUS' ENTERED AT 14:50:09 ON 14 JUN 2006

     FILE 'REGISTRY' ENTERED AT 14:51:48 ON 14 JUN 2006
L68             1 S 119643-83-3/RN
                  SET NOTICE 1 DISPLAY
                  SET NOTICE LOGIN DISPLAY

     FILE 'CAPLUS' ENTERED AT 14:52:04 ON 14 JUN 2006
                  S L57 NOT  119643-82-2/REG#

     FILE 'REGISTRY' ENTERED AT 14:52:47 ON 14 JUN 2006
L69             1 S 119643-82-2/RN

     FILE 'CAPLUS' ENTERED AT 14:52:48 ON 14 JUN 2006
L70            13 S L69
L71           885 S L57 NOT L70
L72             6 S L71 AND PRODRUG
                  S 21919-05-1/REG#

     FILE 'REGISTRY' ENTERED AT 14:54:26 ON 14 JUN 2006
L73             1 S 21919-05-1/RN

     FILE 'CAPLUS' ENTERED AT 14:54:26 ON 14 JUN 2006
L74           176 S L73

=> s l74 or l63
L75           201 L74 OR L63

=> s l75 not l63
L76            23 L75 NOT L63

=> s l76 and l71
L77             0 L76 AND L71

=> s methylnicotinamide
```

```
          1670 METHYLNICOTINAMIDE
            11 METHYLNICOTINAMIDES
L78       1676 METHYLNICOTINAMIDE
                (METHYLNICOTINAMIDE OR METHYLNICOTINAMIDES)

=> s l78 and l75
L79          2 L78 AND L75

=> d ibib 1-2

L79  ANSWER 1 OF 2  CAPLUS  COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER:        1995:620223  CAPLUS
DOCUMENT NUMBER:         123:25632
TITLE:                   Virtual cofactors for an Escherichia coli
                         nitroreductase enzyme: relevance to reductively
                         activated prodrugs in antibody directed enzyme prodrug
                         therapy (ADEPT)
AUTHOR(S):               Knox, Richard J.; Friedlos, Frank; Jarman, Michael;
                         Davies, Lawrence C.; Goddard, Phyllis; Anlezark,
                         Gillian M.; Melton, Roger G.; Sherwood, Roger F.
CORPORATE SOURCE:        Cent. Cancer Therapeutics, Inst. Cancer Res.,
                         Sutton/Surrey, UK
SOURCE:                  Biochemical Pharmacology (1995), 49(11), 1641-7
                         CODEN: BCPCA6; ISSN: 0006-2952
PUBLISHER:               Elsevier
DOCUMENT TYPE:           Journal
LANGUAGE:                English

L79  ANSWER 2 OF 2  CAPLUS  COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER:        1992:566472  CAPLUS
DOCUMENT NUMBER:         117:166472
TITLE:                   Identification of novel reduced pyridinium derivatives
                         as synthetic cofactors for the enzyme DT diaphorase
                         (NAD(P)H dehydrogenase (quinone), EC 1.6.99.2)
AUTHOR(S):               Friedlos, Frank; Jarman, Michael; Davies, Lawrence C.;
                         Boland, Marion P.; Knox, Richard J.
CORPORATE SOURCE:        Sect. Drug Dev., Inst. Cancer Res., Sutton/Surrey, SM2
                         5NG, UK
SOURCE:                  Biochemical Pharmacology (1992), 44(1), 25-31
                         CODEN: BCPCA6; ISSN: 0006-2952
DOCUMENT TYPE:           Journal
LANGUAGE:                English


=> d abs kwic 1-2

L79  ANSWER 1 OF 2  CAPLUS  COPYRIGHT 2006 ACS on STN
AB   A nitroreductase enzyme has been isolated from Escherichia coli that has
     the unusual property of being equally capable of using either NADH or
     NADPH as a cofactor for the reduction of its substrates which include
     menadione as well as 5-(aziridin-1-yl)-2,4-dinitrobenzamide (CB
     1954). This property is shared with the mammalian enzyme, DT
     diaphorase. The nitroreductase can, like DT diaphorase, also use simple
     reduced pyridinium compds. as virtual cofactors. The intact NAD(P)H mol.
     is not required and the simplest quaternary (and therefore reducible)
     derivative of nicotinamide, 1-methylnicotinamide (reduced), is as
     effective as NAD(P)H in its ability to act as an electron donor for the
     nitroreductase. The structure-activity relation is not identical to that
     of DT diaphorase and nicotinic acid riboside (reduced) is selective, being
     active only for the nitroreductase. Irresp. of the virtual cofactor used,
     the nitroreductase formed the same reduction products of CB
     1954 (the 2- and 4-hydroxylamino derivs. in equal proportions).
     Nicotinic acid riboside (reduced), unlike NADH, was stable to metabolism by
     serum enzymes and had a plasma half-life of seven minutes in the mouse
```

after an i.v. bolus administration. NADH had an unmeasurably short half-life. Nicotinic acid riboside (reduced) could also be produced in vivo by administration of nicotinic acid 5'-O-benzoyl riboside (reduced). These results demonstrate that the requirement for a cofactor need not be a limitation in the use of reductive enzymes in antibody directed enzyme prodrug therapy (ADEPT). It is proposed that the E. coli nitroreductase would be a suitable enzyme for ADEPT in combination with **CB 1954** and a synthetic, enzyme-selective, virtual cofactor such as nicotinic acid riboside (reduced).

AB . . . either NADH or NADPH as a cofactor for the reduction of its substrates which include menadione as well as 5-(aziridin-1-yl)-2,4-dinitrobenzamide (**CB 1954**). This property is shared with the mammalian enzyme, DT diaphorase. The nitroreductase can, like DT diaphorase, also use simple reduced. . . as virtual cofactors. The intact NAD(P)H mol. is not required and the simplest quaternary (and therefore reducible) derivative of nicotinamide, 1-**methylnicotinamide** (reduced), is as effective as NAD(P)H in its ability to act as an electron donor for the nitroreductase. The structure-activity. . . being active only for the nitroreductase. Irresp. of the virtual cofactor used, the nitroreductase formed the same reduction products of **CB 1954** (the 2- and 4-hydroxylamino derivs. in equal proportions). Nicotinic acid riboside (reduced), unlike NADH, was stable to metabolism by serum. . . therapy (ADEPT). It is proposed that the E. coli nitroreductase would be a suitable enzyme for ADEPT in combination with **CB 1954** and a synthetic, enzyme-selective, virtual cofactor such as nicotinic acid riboside (reduced).

L79 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN

AB The enzyme DT diaphorase [NAD(P)H dehydrogenase (quinone), EC 1.6.99.2] is unusual in that it can utilize either NADH or NADPH as a cofactor for the reduction of its substrates. It was previously shown that the intact NAD(P)H mol. is not required and that other reduced pyridinium compds. can also act as cofactors for DT diaphorase. The entire adenine dinucleotide portion of NAD(P)H can be dispensed with entirely and the simplest quaternary (and therefore reducible) derivative of nicotinamide, 1-**methylnicotinamide**, was as effective as NAD(P)H as a co-factor for the reduction of the quinone, menadione. Nicotinamide 5'-O-benzoyl riboside was also as effective a cofactor as NAD(P)H, while nicotinamide ribotide and riboside have a higher Km, and decreased kcat with DT diaphorase. Nicotinic acid derivs. had little activity. Kinetic anal. indicated that both nicotinamide ribotide and riboside may be interacting with the menadione binding site rather than the NAD(P)H site. Irresp. of the differences between the various reduced pyridinium derivs. in their ability to act as cofactors for the reduction of menadione by DT diaphorase, all the compds. that showed activity in this assay were equally effective co-factors for the reduction of the nitrobenzamide, **CB 1954** [5-(aziridin-1-yl)-2,4-dinitrobenzamide]. The apparent Km of DT diaphorase for all these cofactors approached zero. It was concluded that cofactor binding is not a rate-limiting step in the nitroreductase activity of DT diaphorase.

AB . . . adenine dinucleotide portion of NAD(P)H can be dispensed with entirely and the simplest quaternary (and therefore reducible) derivative of nicotinamide, 1-**methylnicotinamide**, was as effective as NAD(P)H as a co-factor for the reduction of the quinone, menadione. Nicotinamide 5'-O-benzoyl riboside was also. . . diaphorase, all the compds. that showed activity in this assay were equally effective co-factors for the reduction of the nitrobenzamide, **CB 1954** [5-(aziridin-1-yl)-2,4-dinitrobenzamide]. The apparent Km of DT diaphorase for all these cofactors approached zero. It was concluded that cofactor binding is. . .

IT **21919-05-1**

RL: BIOL (Biological study)
(reaction of DT diaphorase of Walker 256 tumor cells, reduced pyridinium derivs. as cofactors for)

IT 53-57-6, NADPH 58-68-4, NADH 86-08-8, 3-Acetylpyridineadenine dinucleotide 321-02-8, Nicotinic acid ribotide 1094-61-7, Nicotinamide ribotide 1341-23-7, Nicotinamide riboside 3106-60-3, 1-**Methylnicotinamide** 5869-54-5, α-NADH 6704-97-8 17720-18-2 32095-01-5 80658-03-3, α-NADPH 143613-19-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with DT diaphorase of Walker 256 tumor cells, kinetics of)

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---Logging off of STN---

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